Figure 1

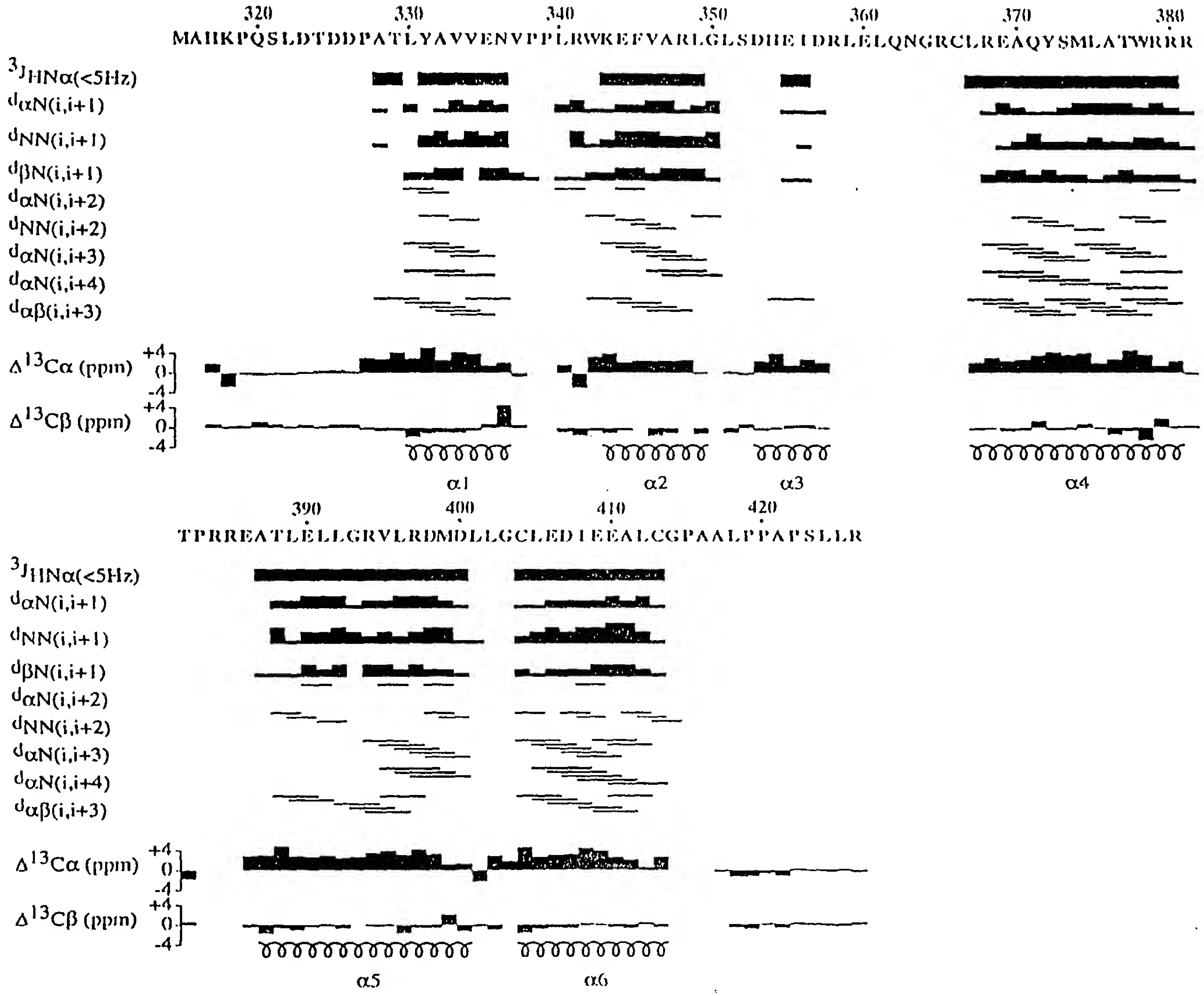

320
330
340
350
360
370
380
MAHKPQSLDTDDPATLYAVVENVPPLRWKEFVARLGLSDHEIDRLELQNGRCLREAQYSMLATWRRR
$^3J_{HN\alpha}$(<5Hz)
$d_{\alpha N}$(i,i+1)
d_{NN}(i,i+1)
$d_{\beta N}$(i,i+1)
$d_{\alpha N}$(i,i+2)
d_{NN}(i,i+2)
$d_{\alpha N}$(i,i+3)
$d_{\alpha N}$(i,i+4)
$d_{\alpha\beta}$(i,i+3)
$\Delta^{13}C\alpha$ (ppm)
+4
0
-4
$\Delta^{13}C\beta$ (ppm)
+4
0
-4
α1
α2
α3
α4
390
400
410
420
TPRREATLELLGRVLRDMDLLGCLEDIEEALCGPAALPPAPSLLR
$^3J_{HN\alpha}$(<5Hz)
$d_{\alpha N}$(i,i+1)
d_{NN}(i,i+1)
$d_{\beta N}$(i,i+1)
$d_{\alpha N}$(i,i+2)
d_{NN}(i,i+2)
$d_{\alpha N}$(i,i+3)
$d_{\alpha N}$(i,i+4)
$d_{\alpha\beta}$(i,i+3)
$\Delta^{13}C\alpha$ (ppm)
+4
0
-4
$\Delta^{13}C\beta$ (ppm)
+4
0
-4
α5
α6

Figure 2

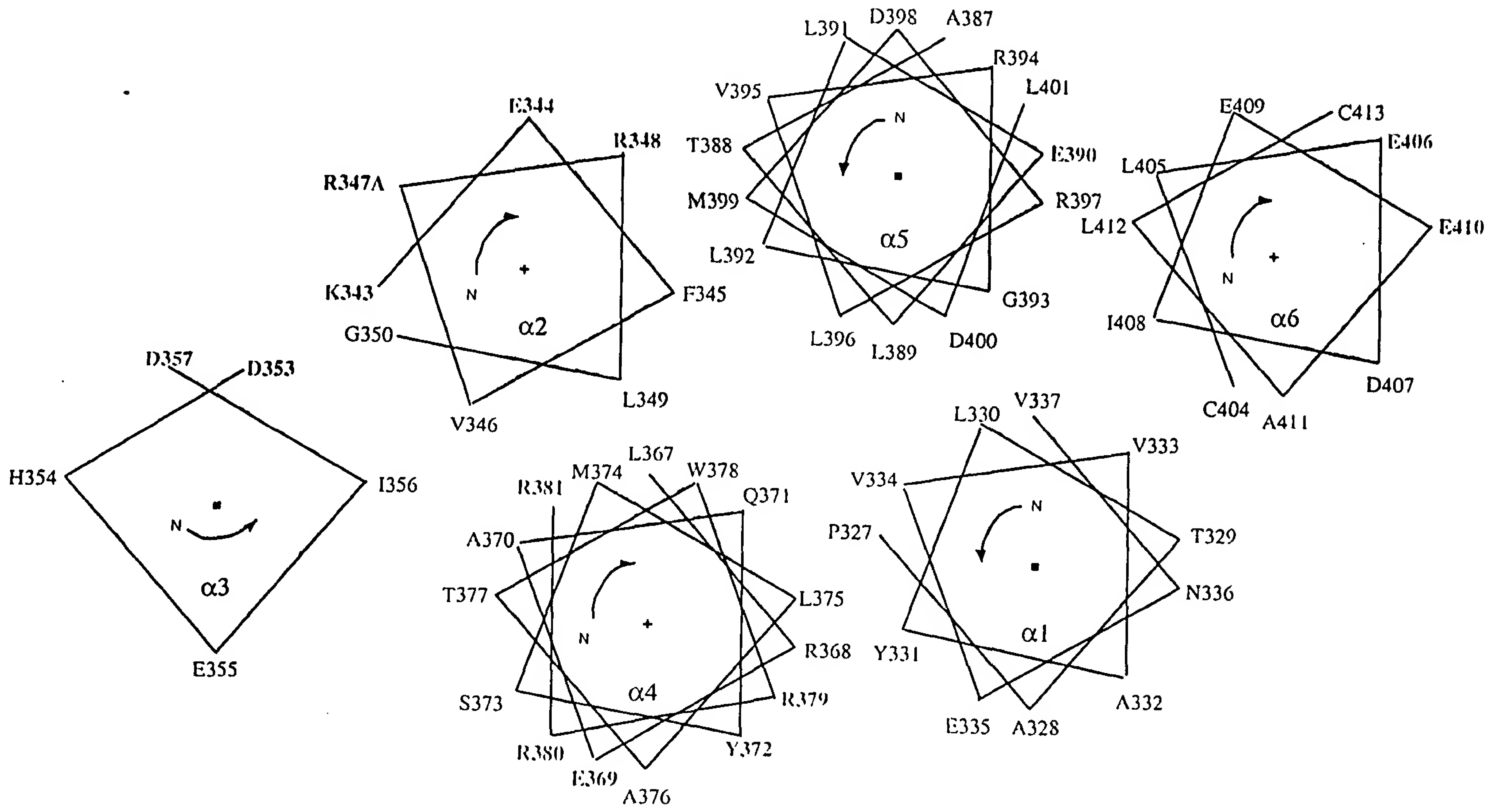

α2
E344
R348
R347A
K343
F345
G350
L349
V346
N
α5
L391
D398
A387
R394
V395
L401
T388
E390
M399
R397
L392
G393
L396
L389
D400
N
α6
E409
C413
E406
L405
L412
E410
I408
D407
C404
A411
N
α3
D357
D353
H354
I356
E355
N
α4
L367
M374
W378
R381
Q371
A370
L375
T377
R368
S373
R379
R380
Y372
E369
A376
N
α1
L330
V337
V333
V334
P327
T329
N336
Y331
E335
A328
A332
N

Figure 3

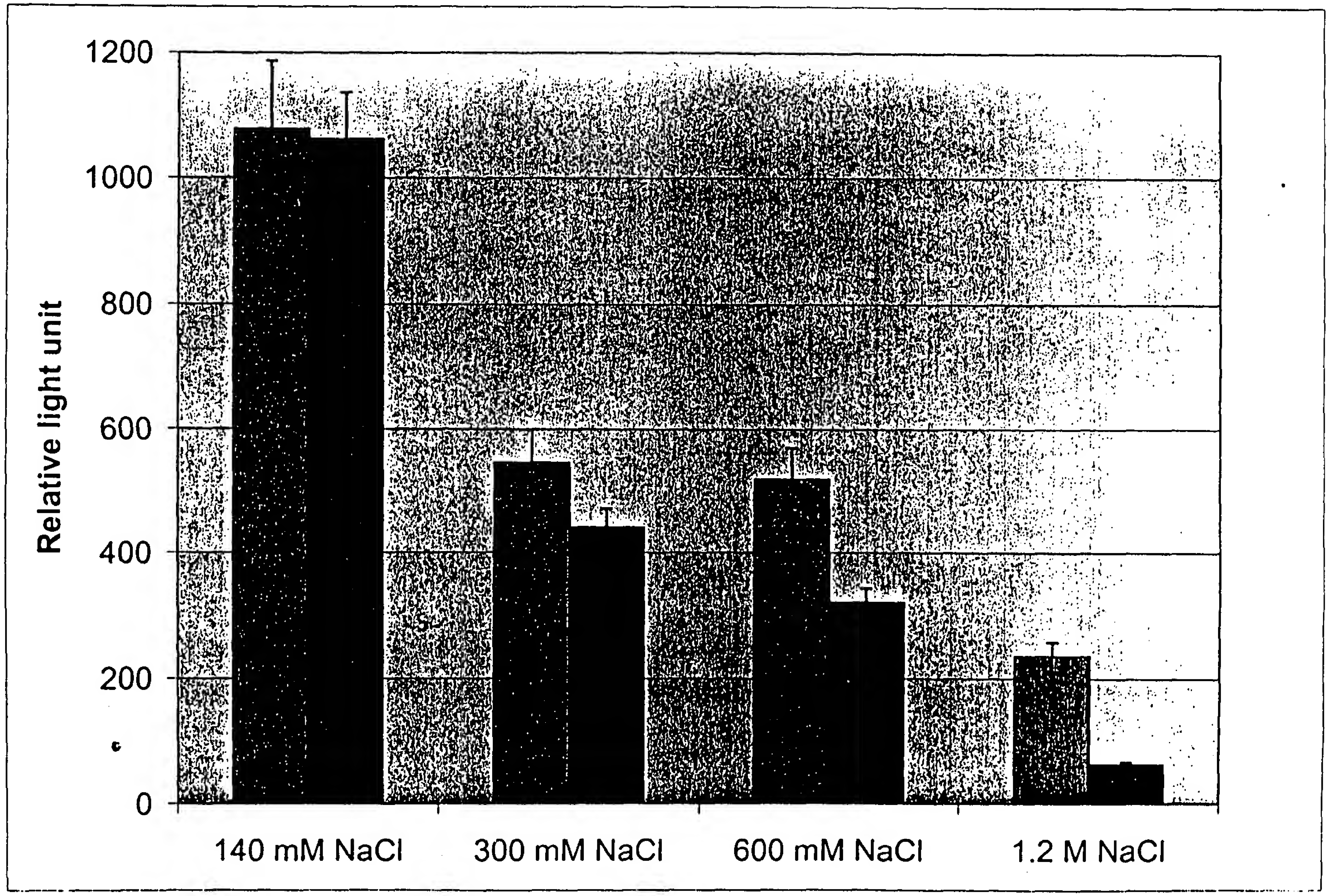
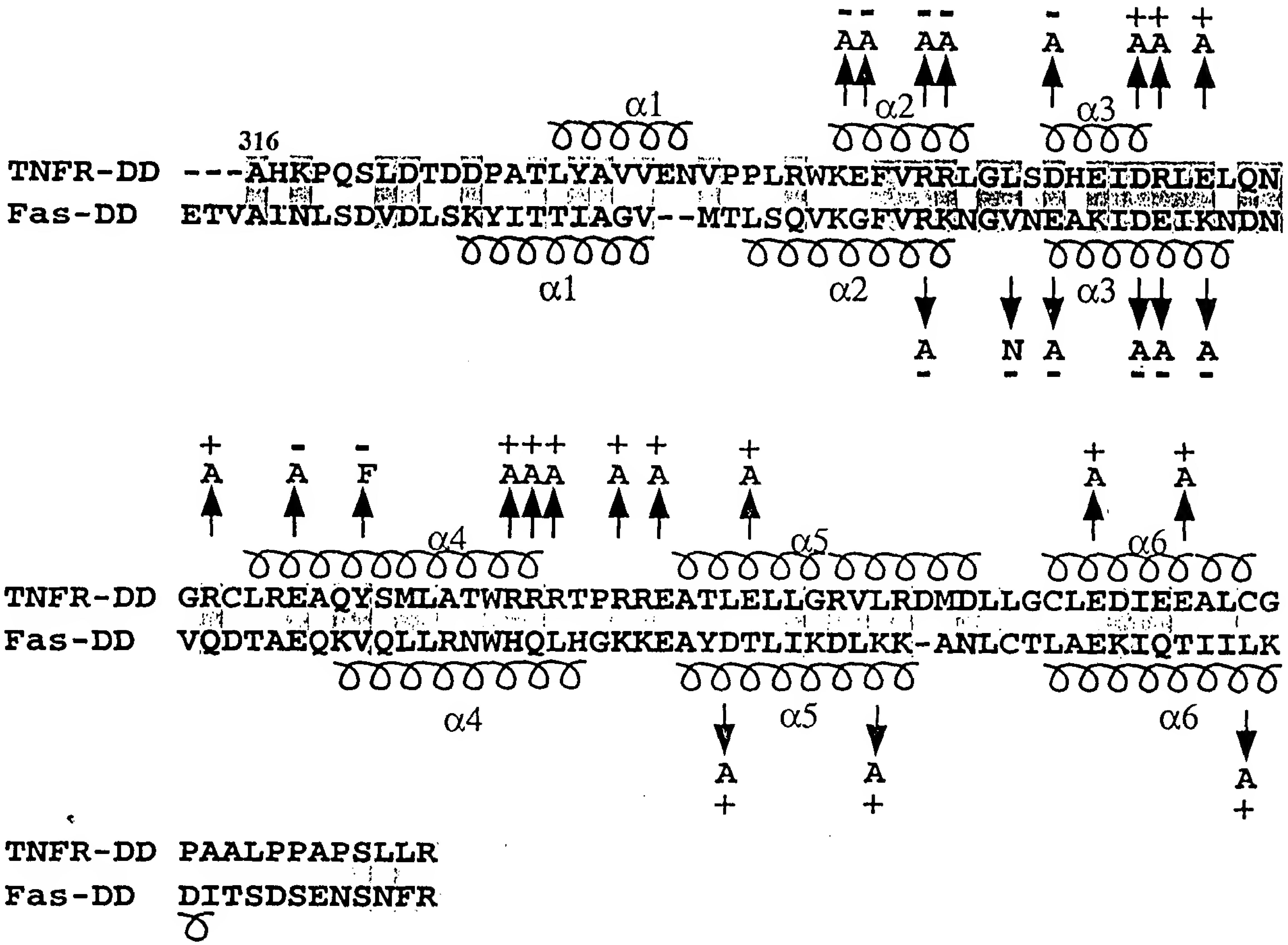

Relative light unit
1200
1000
800
600
400
200
0
140 mM NaCl
300 mM NaCl
600 mM NaCl
1.2 M NaCl

Figure 4



316
TNFR-DD ---AHKPQSLDTDDPATLYAVVENVPPLRWKEFVRRLGLSDHEIDRLELQN
Fas-DD ETVAINLSDVDLSKYITTIAGV--MTLSQVKGFVRKNGVNEAKIDEIKNDN
α1
α2
α3
A
N
F
+
-
TNFR-DD GRCLREAQYSMLATWRRRTPRREATLELLGRVLRDMDLLGCLEDIEEALCG
Fas-DD VQDTAEQKVQLLRNWHQLHGKKEAYDTLIKDLKK-ANLCTLAEKIQTIILK
α4
α5
α6
TNFR-DD PAALPPAPSLLR
Fas-DD DITSDSENSNFR

Figure 5A

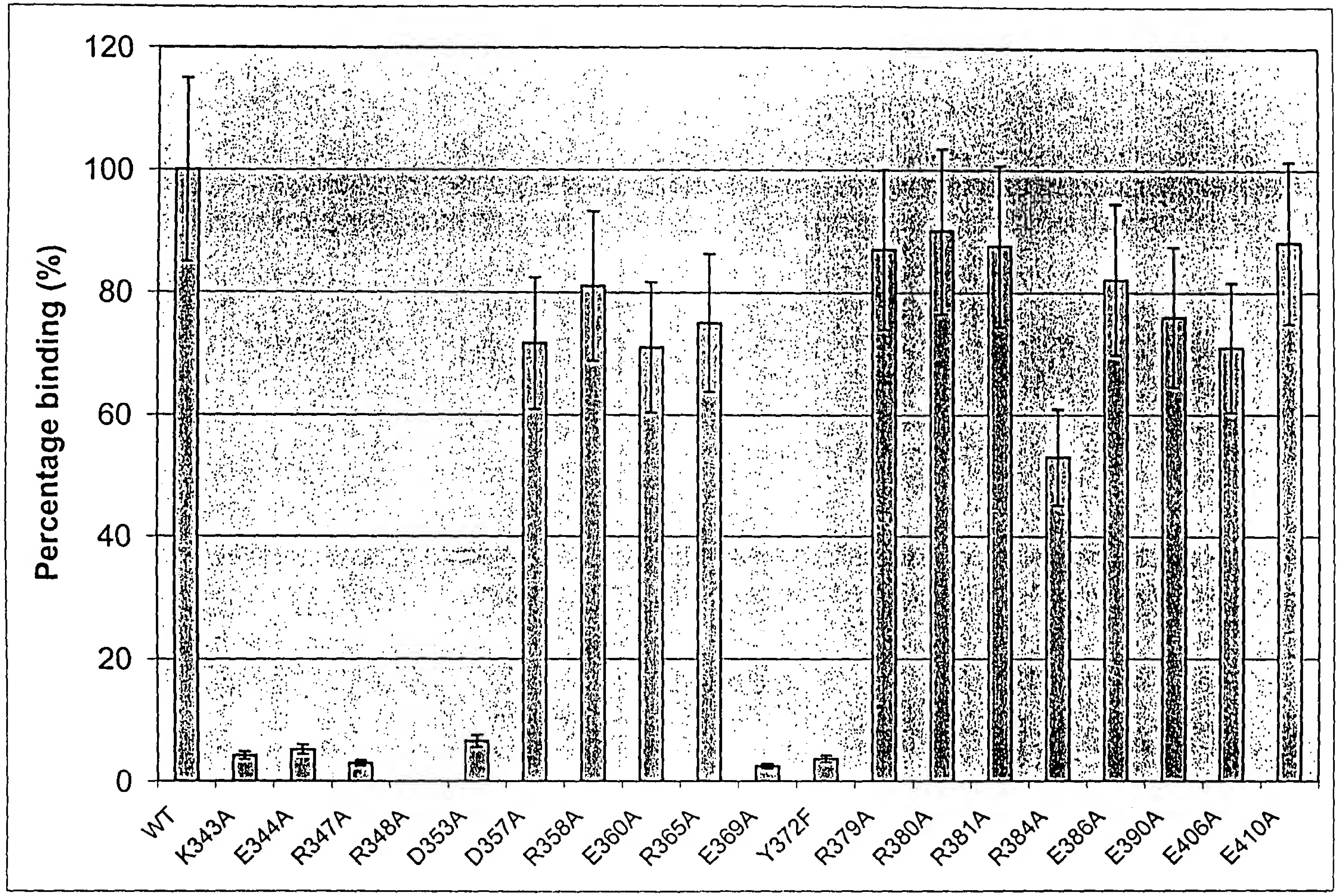

Percentage binding (%)
120
100
80
60
40
20
0
WT
K343A
E344A
R347A
R348A
D353A
D357A
R358A
E360A
R365A
E369A
Y372F
R379A
R380A
R381A
R384A
E386A
E390A
E406A
E410A

Figure 58

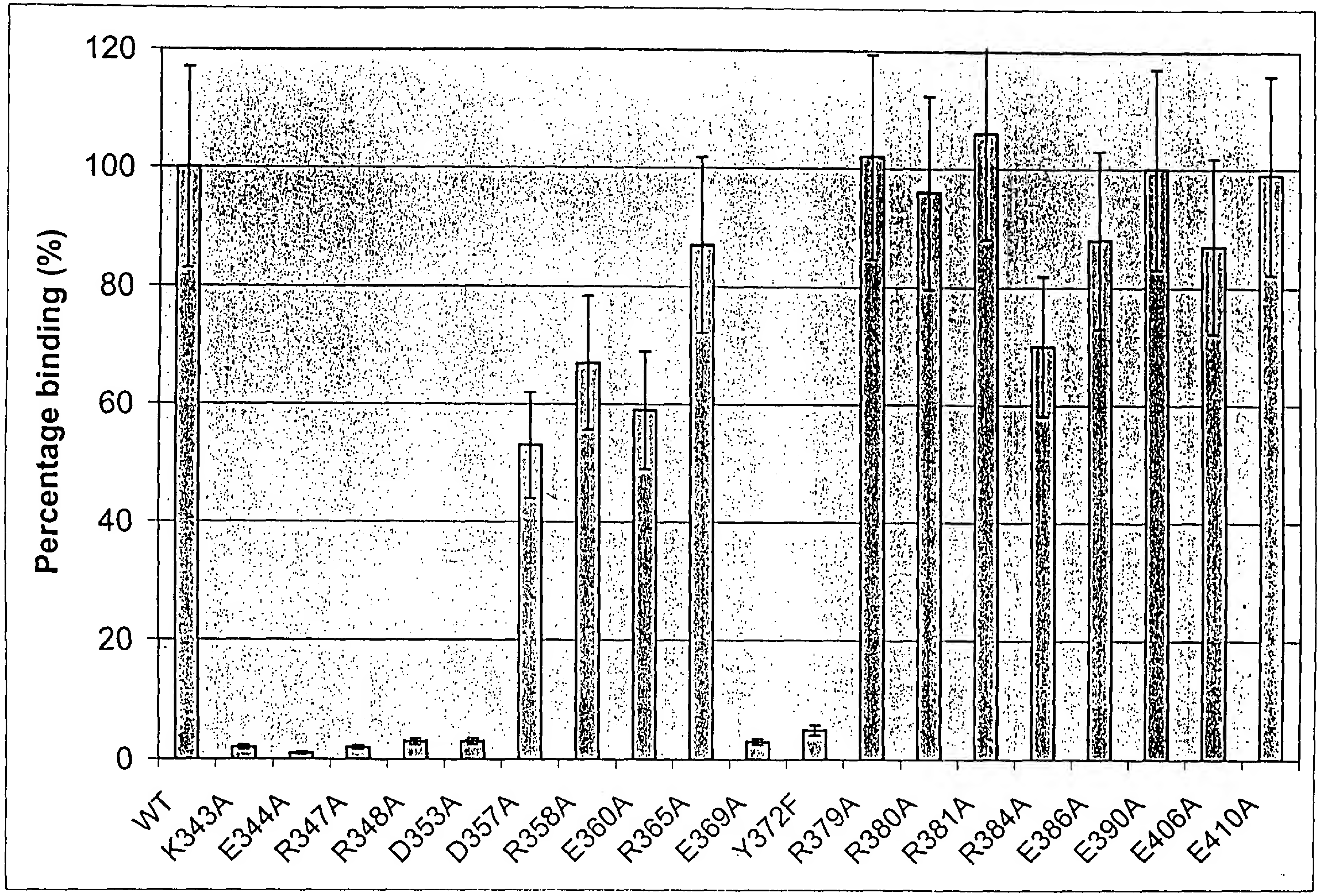
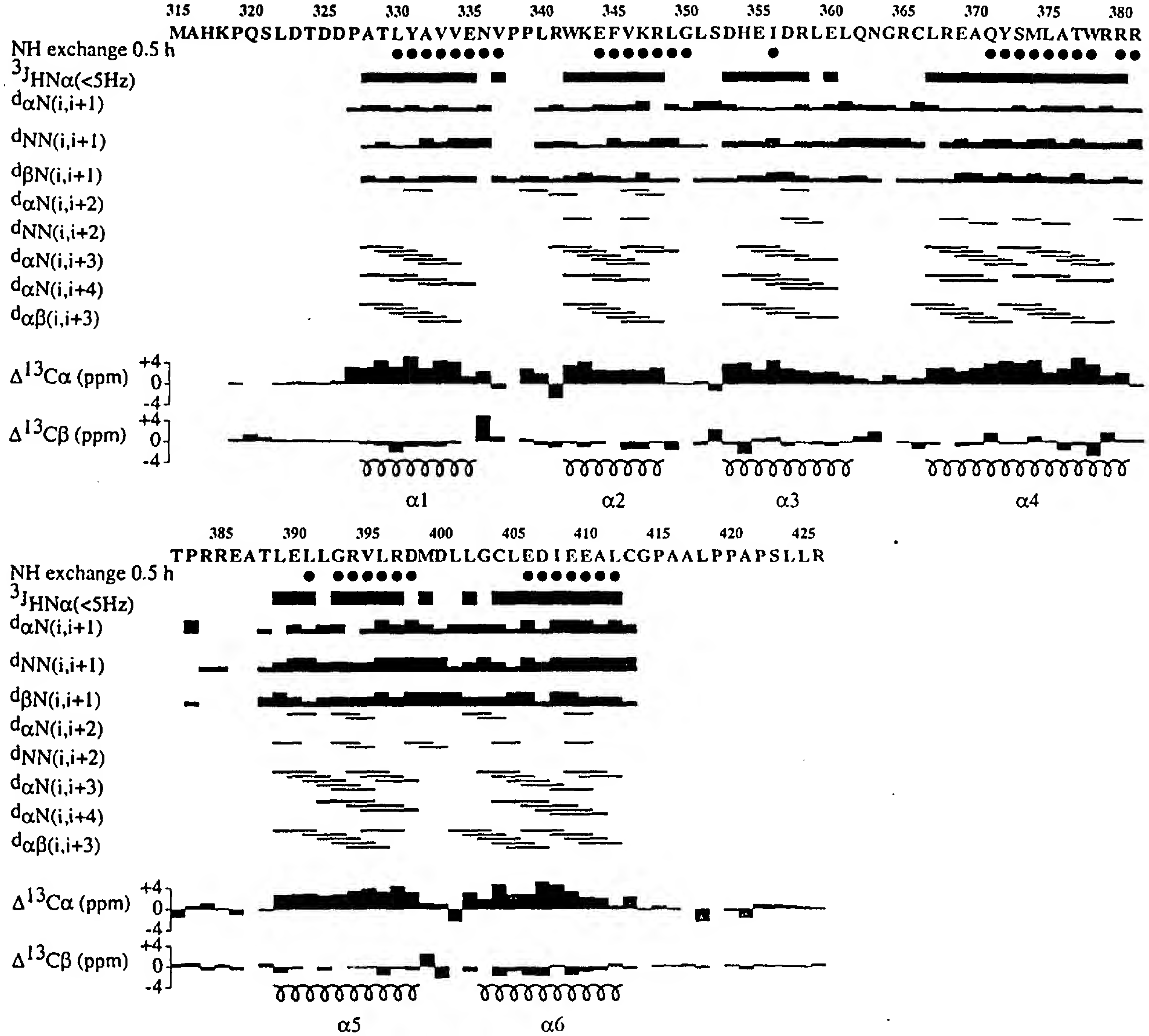
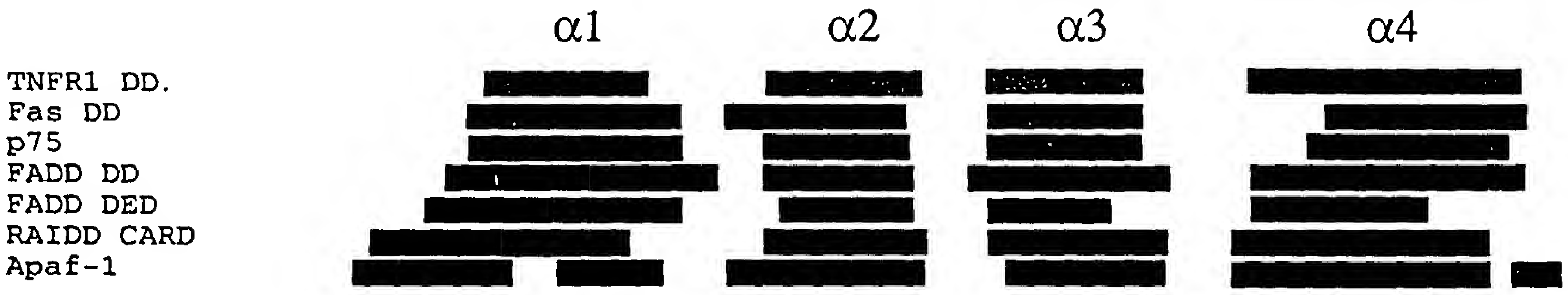

Percentage binding (%)
120
100
80
60
40
20
0
WT
K343A
E344A
R347A
R348A
D353A
D357A
R358A
E360A
R365A
E369A
Y372F
R379A
R380A
R381A
R384A
E386A
E390A
E406A
E410A

Figure 6

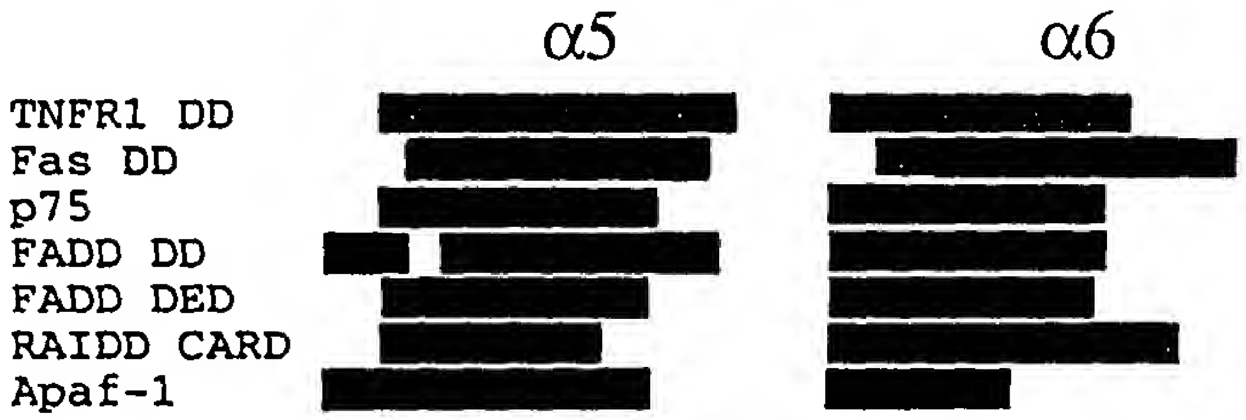


Summary of Secondary Structure Indicators of TNFR-DD R347K

Figure 7



```
TNFR1 DD    MAHKPQSL-DTDDPATLYAVVEN-VPPLRWKE-FVKRLGLSDHEIDRLELQNGRCLREAQYSMLATWRRRTP
Fas DD      METVAINLSDVDLSK--YITTIAGVMTLSQVKGFVRKNGVNEAKIDEIKNDNVQDTAEQKVQLLRNWHQLHG
p75         -----GNLYSSLPLT--KREEVEKLLNGDTWRHLAGELGYQPEHIDSFTHEAC-----PVRALLASWGAQDS
FADD DD     ---GSHMAAPPGEAYLQVAFDIVCDNVGRDWKRLARELKVSEAKMDGIEEKYPRSLSERVRESLKVWKNAEK
FADD DED    ---------MDPFLVLLHSVSSSLSSSELTELKFLCLGRVGKRKLERV-----QSGLDLFSMLLEQNDLEPG
RAIDD CARD -----MEARDKQVLRSLRLELGAEVLVEGLVLQYLYQEGILTENHIQEINAQTTGLRKTMLLLDILPSRGPK
Apaf-1      -----MDAKARNCLLQHREALEKDIK-TSYIMDHMISDGFLTISEEEKVRNEPTQQQRAAMLIKMILKKDND
```



```
TNFR1 DD    RREATLELLGRVLRDMDLLGCLEDIEEALCGPAALPPAPSLLR
Fas DD      KKEAYDTLIKDLKK-ANLCTLAEKIQTIILKDITSDSENSNFRNEIQSLVLE
p75         ATLDALLAALRRIQR---ADIVESLCSE
FADD DD     KNASVAGLVKALRTCRLNLVADLVEEAQES
FADD DED    HTELLRELLASL----RRHDLLRRVDDFELE
RAIDD CARD --AFDTFLDS--LQEF-PWVREKLKKAREEAMTDLPAG
Apaf-1      SYVSFYNALLHEGY----KDLAALLHDGIPVVSSS
```

Figure 8 (1 of 19)

		Atom Type	Residue	Res. No.	X	Y	Z		
ATOM	1	N	PRO	327	2.816	0.502	11.316	1.00	0.61
ATOM	2	CA	PRO	327	2.189	1.819	11.030	1.00	0.60
ATOM	3	HA	PRO	327	1.287	1.695	10.452	1.00	0.62
ATOM	4	CB	PRO	327	1.855	2.377	12.410	1.00	0.69
ATOM	5	HB1	PRO	327	0.841	2.129	12.681	1.00	0.75
ATOM	6	HB2	PRO	327	2.000	3.449	12.426	1.00	0.68
ATOM	7	CG	PRO	327	2.811	1.705	13.337	1.00	0.71
ATOM	8	HG1	PRO	327	2.360	1.585	14.310	1.00	0.79
ATOM	9	HG2	PRO	327	3.718	2.289	13.417	1.00	0.69
ATOM	10	CD	PRO	327	3.114	0.354	12.749	1.00	0.68
ATOM	11	HD2	PRO	327	4.156	0.104	12.897	1.00	0.67
ATOM	12	HD1	PRO	327	2.477	-0.400	13.184	1.00	0.74
ATOM	13	C	PRO	327	3.178	2.733	10.300	1.00	0.51
ATOM	14	O	PRO	327	2.851	3.350	9.306	1.00	0.47
ATOM	15	N	ALA	328	4.385	2.823	10.787	1.00	0.51
ATOM	16	HN	ALA	328	4.629	2.318	11.591	1.00	0.55
ATOM	17	CA	ALA	328	5.393	3.697	10.123	1.00	0.46
ATOM	18	HA	ALA	328	5.006	4.703	10.052	1.00	0.47
ATOM	19	CB	ALA	328	6.684	3.703	10.944	1.00	0.51
ATOM	20	HB1	ALA	328	6.619	4.461	11.711	1.00	1.19
ATOM	21	HB2	ALA	328	7.521	3.917	10.297	1.00	1.04
ATOM	22	HB3	ALA	328	6.823	2.736	11.404	1.00	1.17
ATOM	23	C	ALA	328	5.685	3.165	8.720	1.00	0.39
ATOM	24	O	ALA	328	5.930	3.920	7.799	1.00	0.36
ATOM	25	N	THR	329	5.660	1.872	8.545	1.00	0.37
ATOM	26	HN	THR	329	5.459	1.278	9.298	1.00	0.40
ATOM	27	CA	THR	329	5.935	1.303	7.196	1.00	0.34
ATOM	28	HA	THR	329	6.871	1.692	6.823	1.00	0.34
ATOM	29	CB	THR	329	6.012	-0.222	7.279	1.00	0.37
ATOM	30	HB	THR	329	5.045	-0.618	7.549	1.00	0.40
ATOM	31	OG1	THR	329	6.971	-0.601	8.256	1.00	0.39
ATOM	32	HG1	THR	329	6.878	-0.012	9.009	1.00	0.80
ATOM	33	CG2	THR	329	6.419	-0.779	5.915	1.00	0.38
ATOM	34	HG21	THR	329	6.796	0.023	5.297	1.00	1.08
ATOM	35	HG22	THR	329	5.559	-1.226	5.438	1.00	1.05
ATOM	36	HG23	THR	329	7.188	-1.525	6.044	1.00	1.09
ATOM	37	C	THR	329	4.804	1.694	6.247	1.00	0.32
ATOM	38	O	THR	329	4.984	1.773	5.048	1.00	0.30
ATOM	39	N	LEU	330	3.638	1.938	6.776	1.00	0.35
ATOM	40	HN	LEU	330	3.515	1.868	7.745	1.00	0.39
ATOM	41	CA	LEU	330	2.495	2.322	5.905	1.00	0.36
ATOM	42	HA	LEU	330	2.474	1.678	5.038	1.00	0.36
ATOM	43	CB	LEU	330	1.175	2.181	6.678	1.00	0.43
ATOM	44	HB1	LEU	330	0.356	2.118	5.977	1.00	0.71
ATOM	45	HB2	LEU	330	1.038	3.047	7.309	1.00	0.48
ATOM	46	CG	LEU	330	1.193	0.915	7.550	1.00	0.70
ATOM	47	HG	LEU	330	1.892	1.049	8.362	1.00	1.17
ATOM	48	CD1	LEU	330	-0.204	0.675	8.123	1.00	1.17
ATOM	49	HD11	LEU	330	-0.847	1.504	7.863	1.00	1.71
ATOM	50	HD12	LEU	330	-0.142	0.591	9.198	1.00	1.79
ATOM	51	HD13	LEU	330	-0.610	-0.238	7.713	1.00	1.63
ATOM	52	CD2	LEU	330	1.609	-0.300	6.710	1.00	1.69
ATOM	53	HD21	LEU	330	1.114	-0.263	5.752	1.00	2.25
ATOM	54	HD22	LEU	330	1.327	-1.206	7.226	1.00	2.18
ATOM	55	HD23	LEU	330	2.679	-0.287	6.563	1.00	2.16
ATOM	56	C	LEU	330	2.677	3.771	5.454	1.00	0.33
ATOM	57	O	LEU	330	2.472	4.104	4.305	1.00	0.30
ATOM	58	N	TYR	331	3.074	4.636	6.348	1.00	0.35
ATOM	59	HN	TYR	331	3.244	4.347	7.270	1.00	0.38
ATOM	60	CA	TYR	331	3.281	6.059	5.962	1.00	0.36
ATOM	61	HA	TYR	331	2.368	6.457	5.544	1.00	0.37
ATOM	62	CB	TYR	331	3.681	6.872	7.195	1.00	0.42
ATOM	63	HB1	TYR	331	3.987	7.861	6.889	1.00	0.43
ATOM	64	HB2	TYR	331	4.500	6.381	7.699	1.00	0.42
ATOM	65	CG	TYR	331	2.504	6.979	8.134	1.00	0.48
ATOM	66	CD1	TYR	331	1.305	7.551	7.692	1.00	1.26
ATOM	67	HD1	TYR	331	1.221	7.915	6.679	1.00	2.13
ATOM	68	CD2	TYR	331	2.612	6.507	9.448	1.00	1.36
ATOM	69	HD2	TYR	331	3.538	6.066	9.789	1.00	2.24
ATOM	70	CE1	TYR	331	0.214	7.650	8.564	1.00	1.30
ATOM	71	HE1	TYR	331	-0.711	8.091	8.223	1.00	2.18
ATOM	72	CE2	TYR	331	1.521	6.607	10.320	1.00	1.38
ATOM	73	HE2	TYR	331	1.605	6.243	11.333	1.00	2.26
ATOM	74	CZ	TYR	331	0.322	7.178	9.878	1.00	0.63
ATOM	75	OH	TYR	331	-0.753	7.276	10.737	1.00	0.71
ATOM	76	HH	TYR	331	-0.454	7.713	11.538	1.00	1.10
ATOM	77	C	TYR	331	4.396	6.132	4.920	1.00	0.32

```
ATOM     78  O    TYR   331       4.401   6.986   4.055  1.00  0.33
ATOM     79  N    ALA   332       5.340   5.235   4.995  1.00  0.31
ATOM     80  HN   ALA   332       5.312   4.555   5.700  1.00  0.33
ATOM     81  CA   ALA   332       6.456   5.241   4.011  1.00  0.31
ATOM     82  HA   ALA   332       6.880   6.232   3.950  1.00  0.35
ATOM     83  CB   ALA   332       7.532   4.247   4.454  1.00  0.35
ATOM     84  HB1  ALA   332       7.081   3.281   4.628  1.00  1.08
ATOM     85  HB2  ALA   332       7.996   4.597   5.363  1.00  0.98
ATOM     86  HB3  ALA   332       8.279   4.160   3.680  1.00  1.12
ATOM     87  C    ALA   332       5.922   4.826   2.642  1.00  0.28
ATOM     88  O    ALA   332       6.274   5.395   1.629  1.00  0.31
ATOM     89  N    VAL   333       5.077   3.832   2.604  1.00  0.26
ATOM     90  HN   VAL   333       4.809   3.385   3.434  1.00  0.27
ATOM     91  CA   VAL   333       4.525   3.374   1.300  1.00  0.26
ATOM     92  HA   VAL   333       5.335   3.242   0.597  1.00  0.29
ATOM     93  CB   VAL   333       3.803   2.040   1.496  1.00  0.28
ATOM     94  HB   VAL   333       3.015   2.161   2.225  1.00  0.27
ATOM     95  CG1  VAL   333       3.202   1.576   0.167  1.00  0.30
ATOM     96  HG11 VAL   333       2.209   1.186   0.338  1.00  1.07
ATOM     97  HG12 VAL   333       3.823   0.802  -0.258  1.00  1.01
ATOM     98  HG13 VAL   333       3.148   2.409  -0.517  1.00  1.09
ATOM     99  CG2  VAL   333       4.803   0.993   1.992  1.00  0.33
ATOM    100  HG21 VAL   333       5.237   0.480   1.146  1.00  1.10
ATOM    101  HG22 VAL   333       4.295   0.279   2.623  1.00  1.02
ATOM    102  HG23 VAL   333       5.584   1.481   2.556  1.00  1.07
ATOM    103  C    VAL   333       3.547   4.419   0.756  1.00  0.24
ATOM    104  O    VAL   333       3.562   4.741  -0.416  1.00  0.27
ATOM    105  N    VAL   334       2.696   4.953   1.590  1.00  0.22
ATOM    106  HN   VAL   334       2.694   4.685   2.532  1.00  0.22
ATOM    107  CA   VAL   334       1.726   5.973   1.098  1.00  0.25
ATOM    108  HA   VAL   334       1.127   5.544   0.310  1.00  0.29
ATOM    109  CB   VAL   334       0.812   6.420   2.244  1.00  0.29
ATOM    110  HB   VAL   334       1.410   6.823   3.048  1.00  0.30
ATOM    111  CG1  VAL   334      -0.151   7.491   1.735  1.00  0.40
ATOM    112  HG11 VAL   334      -0.343   7.329   0.685  1.00  1.10
ATOM    113  HG12 VAL   334       0.289   8.467   1.876  1.00  1.09
ATOM    114  HG13 VAL   334      -1.079   7.430   2.284  1.00  1.01
ATOM    115  CG2  VAL   334      -0.001   5.228   2.752  1.00  0.36
ATOM    116  HG21 VAL   334      -0.571   4.808   1.936  1.00  1.12
ATOM    117  HG22 VAL   334      -0.675   5.559   3.529  1.00  1.08
ATOM    118  HG23 VAL   334       0.666   4.480   3.149  1.00  0.97
ATOM    119  C    VAL   334       2.491   7.182   0.550  1.00  0.27
ATOM    120  O    VAL   334       2.024   7.874  -0.332  1.00  0.32
ATOM    121  N    GLU   335       3.661   7.443   1.067  1.00  0.31
ATOM    122  HN   GLU   335       4.021   6.874   1.779  1.00  0.35
ATOM    123  CA   GLU   335       4.450   8.608   0.573  1.00  0.38
ATOM    124  HA   GLU   335       3.776   9.380   0.231  1.00  0.40
ATOM    125  CB   GLU   335       5.316   9.155   1.710  1.00  0.41
ATOM    126  HB1  GLU   335       6.358   9.090   1.433  1.00  0.99
ATOM    127  HB2  GLU   335       5.144   8.574   2.604  1.00  1.01
ATOM    128  CG   GLU   335       4.951  10.617   1.971  1.00  1.26
ATOM    129  HG1  GLU   335       3.896  10.691   2.188  1.00  1.99
ATOM    130  HG2  GLU   335       5.181  11.207   1.095  1.00  1.84
ATOM    131  CD   GLU   335       5.752  11.139   3.165  1.00  1.56
ATOM    132  OE1  GLU   335       5.139  11.659   4.082  1.00  2.26
ATOM    133  OE2  GLU   335       6.965  11.009   3.141  1.00  1.81
ATOM    134  C    GLU   335       5.350   8.168  -0.584  1.00  0.41
ATOM    135  O    GLU   335       5.396   8.797  -1.623  1.00  0.48
ATOM    136  N    ASN   336       6.069   7.093  -0.411  1.00  0.41
ATOM    137  HN   ASN   336       6.019   6.603   0.436  1.00  0.39
ATOM    138  CA   ASN   336       6.970   6.612  -1.497  1.00  0.47
ATOM    139  HA   ASN   336       7.711   7.366  -1.712  1.00  0.53
ATOM    140  CB   ASN   336       7.665   5.327  -1.046  1.00  0.50
ATOM    141  HB1  ASN   336       7.812   4.680  -1.897  1.00  0.68
ATOM    142  HB2  ASN   336       7.052   4.824  -0.314  1.00  0.81
ATOM    143  CG   ASN   336       9.021   5.670  -0.429  1.00  0.81
ATOM    144  OD1  ASN   336      10.034   5.130  -0.825  1.00  1.73
ATOM    145  ND2  ASN   336       9.084   6.551   0.531  1.00  1.22
ATOM    146  HD21 ASN   336       8.266   6.986   0.851  1.00  1.80
ATOM    147  HD22 ASN   336       9.949   6.777   0.933  1.00  1.52
ATOM    148  C    ASN   336       6.156   6.334  -2.758  1.00  0.45
ATOM    149  O    ASN   336       6.262   7.036  -3.744  1.00  0.53
ATOM    150  N    VAL   337       5.347   5.312  -2.739  1.00  0.36
ATOM    151  HN   VAL   337       5.277   4.755  -1.936  1.00  0.32
ATOM    152  CA   VAL   337       4.534   4.992  -3.943  1.00  0.36
ATOM    153  HA   VAL   337       5.192   4.703  -4.748  1.00  0.41
ATOM    154  CB   VAL   337       3.585   3.838  -3.623  1.00  0.32
```

```
ATOM    155  HB  VAL   337       2.904   4.137  -2.841  1.00  0.33
ATOM    156  CG1 VAL   337       2.791   3.468  -4.877  1.00  0.36
ATOM    157 HG11 VAL   337       2.519   4.368  -5.408  1.00  1.01
ATOM    158 HG12 VAL   337       1.898   2.933  -4.592  1.00  1.05
ATOM    159 HG13 VAL   337       3.398   2.843  -5.515  1.00  1.08
ATOM    160  CG2 VAL   337       4.398   2.626  -3.161  1.00  0.36
ATOM    161 HG21 VAL   337       5.411   2.933  -2.948  1.00  1.07
ATOM    162 HG22 VAL   337       4.404   1.879  -3.940  1.00  1.10
ATOM    163 HG23 VAL   337       3.952   2.213  -2.269  1.00  1.07
ATOM    164  C   VAL   337       3.721   6.228  -4.353  1.00  0.43
ATOM    165  O   VAL   337       3.120   6.872  -3.517  1.00  0.44
ATOM    166  N   PRO   338       3.726   6.524  -5.631  1.00  0.51
ATOM    167  CA  PRO   338       2.973   7.700  -6.137  1.00  0.62
ATOM    168  HA  PRO   338       3.272   8.592  -5.611  1.00  0.65
ATOM    169  CB  PRO   338       3.393   7.792  -7.603  1.00  0.71
ATOM    170  HB1 PRO   338       4.218   8.477  -7.717  1.00  0.78
ATOM    171  HB2 PRO   338       2.556   8.101  -8.214  1.00  0.77
ATOM    172  CG  PRO   338       3.823   6.408  -7.962  1.00  0.64
ATOM    173  HG1 PRO   338       4.570   6.440  -8.740  1.00  0.71
ATOM    174  HG2 PRO   338       2.970   5.828  -8.287  1.00  0.63
ATOM    175  CD  PRO   338       4.415   5.810  -6.714  1.00  0.53
ATOM    176  HD2 PRO   338       4.209   4.749  -6.666  1.00  0.48
ATOM    177  HD1 PRO   338       5.476   5.997  -6.666  1.00  0.58
ATOM    178  C   PRO   338       1.460   7.465  -6.006  1.00  0.63
ATOM    179  O   PRO   338       0.977   6.393  -6.311  1.00  0.62
ATOM    180  N   PRO   339       0.758   8.476  -5.549  1.00  0.70
ATOM    181  CA  PRO   339      -0.712   8.361  -5.375  1.00  0.76
ATOM    182  HA  PRO   339      -0.965   7.452  -4.855  1.00  0.72
ATOM    183  CB  PRO   339      -1.066   9.568  -4.514  1.00  0.82
ATOM    184  HB1 PRO   339      -1.075   9.296  -3.470  1.00  0.77
ATOM    185  HB2 PRO   339      -2.027   9.967  -4.808  1.00  0.91
ATOM    186  CG  PRO   339       0.015  10.568  -4.772  1.00  0.87
ATOM    187  HG1 PRO   339       0.205  11.144  -3.880  1.00  0.89
ATOM    188  HG2 PRO   339      -0.278  11.224  -5.580  1.00  0.98
ATOM    189  CD  PRO   339       1.255   9.803  -5.154  1.00  0.78
ATOM    190  HD2 PRO   339       1.756  10.285  -5.982  1.00  0.85
ATOM    191  HD1 PRO   339       1.920   9.713  -4.309  1.00  0.76
ATOM    192  C   PRO   339      -1.443   8.438  -6.723  1.00  0.90
ATOM    193  O   PRO   339      -2.655   8.373  -6.780  1.00  1.13
ATOM    194  N   LEU   340      -0.728   8.587  -7.805  1.00  0.99
ATOM    195  HN  LEU   340       0.247   8.647  -7.749  1.00  1.13
ATOM    196  CA  LEU   340      -1.406   8.677  -9.129  1.00  1.11
ATOM    197  HA  LEU   340      -2.269   9.321  -9.045  1.00  1.47
ATOM    198  CB  LEU   340      -0.439   9.262 -10.161  1.00  1.35
ATOM    199  HB1 LEU   340       0.311   8.527 -10.409  1.00  1.21
ATOM    200  HB2 LEU   340       0.039  10.140  -9.749  1.00  1.73
ATOM    201  CG  LEU   340      -1.213   9.646 -11.424  1.00  1.45
ATOM    202  HG  LEU   340      -1.677   8.764 -11.842  1.00  1.29
ATOM    203  CD1 LEU   340      -2.293  10.670 -11.071  1.00  1.81
ATOM    204 HD11 LEU   340      -1.936  11.311 -10.279  1.00  2.38
ATOM    205 HD12 LEU   340      -3.184  10.156 -10.744  1.00  1.87
ATOM    206 HD13 LEU   340      -2.521  11.267 -11.942  1.00  2.04
ATOM    207  CD2 LEU   340      -0.251  10.253 -12.447  1.00  1.78
ATOM    208 HD21 LEU   340       0.768  10.053 -12.147  1.00  1.70
ATOM    209 HD22 LEU   340      -0.408  11.320 -12.500  1.00  2.32
ATOM    210 HD23 LEU   340      -0.433   9.814 -13.417  1.00  2.30
ATOM    211  C   LEU   340      -1.855   7.287  -9.585  1.00  0.73
ATOM    212  O   LEU   340      -2.990   7.089  -9.972  1.00  0.98
ATOM    213  N   ARG   341      -0.975   6.325  -9.555  1.00  0.40
ATOM    214  HN  ARG   341      -0.062   6.505  -9.247  1.00  0.41
ATOM    215  CA  ARG   341      -1.356   4.953 -10.000  1.00  0.68
ATOM    216  HA  ARG   341      -2.323   4.986 -10.480  1.00  0.99
ATOM    217  CB  ARG   341      -0.311   4.433 -10.993  1.00  1.12
ATOM    218  HB1 ARG   341      -0.378   3.357 -11.054  1.00  1.46
ATOM    219  HB2 ARG   341       0.676   4.713 -10.654  1.00  1.51
ATOM    220  CG  ARG   341      -0.566   5.037 -12.380  1.00  1.89
ATOM    221  HG1 ARG   341      -1.485   4.639 -12.782  1.00  2.12
ATOM    222  HG2 ARG   341       0.253   4.784 -13.038  1.00  2.27
ATOM    223  CD  ARG   341      -0.679   6.562 -12.269  1.00  2.83
ATOM    224  HD1 ARG   341       0.021   6.919 -11.526  1.00  3.07
ATOM    225  HD2 ARG   341      -1.684   6.822 -11.966  1.00  2.89
ATOM    226  NE  ARG   341      -0.375   7.186 -13.589  1.00  3.77
ATOM    227  HE  ARG   341      -1.083   7.281 -14.260  1.00  3.89
ATOM    228  CZ  ARG   341       0.832   7.609 -13.851  1.00  4.65
ATOM    229  NH1 ARG   341       1.861   7.057 -13.266  1.00  5.32
ATOM    230 HH11 ARG   341       1.726   6.310 -12.616  1.00  5.28
ATOM    231 HH12 ARG   341       2.785   7.382 -13.469  1.00  6.08
```

```
ATOM    232  NH2 ARG   341       1.011   8.584 -14.701  1.00  5.18
ATOM    233 HH21 ARG   341       0.223   9.006 -15.149  1.00  5.01
ATOM    234 HH22 ARG   341       1.935   8.909 -14.903  1.00  5.96
ATOM    235  C   ARG   341      -1.421   4.033  -8.790  1.00  0.54
ATOM    236  O   ARG   341      -1.148   2.852  -8.872  1.00  0.50
ATOM    237  N   TRP   342      -1.781   4.573  -7.662  1.00  0.53
ATOM    238  HN  TRP   342      -1.991   5.532  -7.631  1.00  0.61
ATOM    239  CA  TRP   342      -1.866   3.740  -6.426  1.00  0.42
ATOM    240  HA  TRP   342      -0.870   3.445  -6.127  1.00  0.43
ATOM    241  CB  TRP   342      -2.513   4.543  -5.295  1.00  0.43
ATOM    242  HB1 TRP   342      -3.557   4.705  -5.518  1.00  0.47
ATOM    243  HB2 TRP   342      -2.011   5.494  -5.194  1.00  0.50
ATOM    244  CG  TRP   342      -2.387   3.771  -4.022  1.00  0.34
ATOM    245  CD1 TRP   342      -3.270   2.845  -3.583  1.00  0.35
ATOM    246  HD1 TRP   342      -4.177   2.553  -4.091  1.00  0.42
ATOM    247  CD2 TRP   342      -1.330   3.834  -3.021  1.00  0.30
ATOM    248  NE1 TRP   342      -2.819   2.332  -2.380  1.00  0.31
ATOM    249  HE1 TRP   342      -3.276   1.644  -1.853  1.00  0.35
ATOM    250  CE2 TRP   342      -1.628   2.911  -1.991  1.00  0.28
ATOM    251  CE3 TRP   342      -0.153   4.595  -2.910  1.00  0.34
ATOM    252  HE3 TRP   342       0.100   5.308  -3.681  1.00  0.39
ATOM    253  CZ2 TRP   342      -0.785   2.747  -0.889  1.00  0.31
ATOM    254  HZ2 TRP   342      -1.030   2.032  -0.116  1.00  0.35
ATOM    255  CZ3 TRP   342       0.695   4.435  -1.803  1.00  0.37
ATOM    256  HZ3 TRP   342       1.595   5.026  -1.727  1.00  0.44
ATOM    257  CH2 TRP   342       0.380   3.513  -0.795  1.00  0.35
ATOM    258  HH2 TRP   342       1.036   3.397   0.055  1.00  0.42
ATOM    259  C   TRP   342      -2.701   2.485  -6.700  1.00  0.35
ATOM    260  O   TRP   342      -2.269   1.378  -6.444  1.00  0.34
ATOM    261  N   LYS   343      -3.892   2.646  -7.223  1.00  0.36
ATOM    262  HN  LYS   343      -4.218   3.548  -7.425  1.00  0.41
ATOM    263  CA  LYS   343      -4.755   1.458  -7.518  1.00  0.34
ATOM    264  HA  LYS   343      -5.115   1.032  -6.589  1.00  0.35
ATOM    265  CB  LYS   343      -5.946   1.892  -8.375  1.00  0.40
ATOM    266  HB1 LYS   343      -5.592   2.240  -9.334  1.00  0.41
ATOM    267  HB2 LYS   343      -6.478   2.689  -7.875  1.00  0.47
ATOM    268  CG  LYS   343      -6.885   0.702  -8.583  1.00  0.43
ATOM    269  HG1 LYS   343      -7.307   0.406  -7.634  1.00  0.48
ATOM    270  HG2 LYS   343      -6.330  -0.124  -9.004  1.00  0.40
ATOM    271  CD  LYS   343      -8.012   1.099  -9.537  1.00  0.50
ATOM    272  HD1 LYS   343      -7.664   1.024 -10.557  1.00  0.70
ATOM    273  HD2 LYS   343      -8.315   2.116  -9.333  1.00  0.82
ATOM    274  CE  LYS   343      -9.203   0.161  -9.337  1.00  0.87
ATOM    275  HE1 LYS   343      -9.772   0.479  -8.476  1.00  1.44
ATOM    276  HE2 LYS   343      -8.846  -0.846  -9.181  1.00  1.38
ATOM    277  NZ  LYS   343     -10.073   0.197 -10.547  1.00  1.58
ATOM    278  HZ1 LYS   343     -10.202   1.183 -10.852  1.00  2.04
ATOM    279  HZ2 LYS   343     -10.999  -0.221 -10.321  1.00  2.03
ATOM    280  HZ3 LYS   343      -9.625  -0.345 -11.313  1.00  2.15
ATOM    281  C   LYS   343      -3.939   0.407  -8.273  1.00  0.34
ATOM    282  O   LYS   343      -3.994  -0.768  -7.971  1.00  0.36
ATOM    283  N   GLU   344      -3.160   0.822  -9.238  1.00  0.38
ATOM    284  HN  GLU   344      -3.111   1.776  -9.456  1.00  0.40
ATOM    285  CA  GLU   344      -2.324  -0.160  -9.981  1.00  0.44
ATOM    286  HA  GLU   344      -2.959  -0.886 -10.469  1.00  0.47
ATOM    287  CB  GLU   344      -1.472   0.570 -11.021  1.00  0.53
ATOM    288  HB1 GLU   344      -0.656  -0.066 -11.329  1.00  0.90
ATOM    289  HB2 GLU   344      -1.077   1.478 -10.588  1.00  0.68
ATOM    290  CG  GLU   344      -2.333   0.916 -12.237  1.00  1.19
ATOM    291  HG1 GLU   344      -2.676   1.936 -12.157  1.00  1.51
ATOM    292  HG2 GLU   344      -3.184   0.251 -12.276  1.00  1.62
ATOM    293  CD  GLU   344      -1.502   0.759 -13.512  1.00  1.27
ATOM    294  OE1 GLU   344      -0.287   0.793 -13.412  1.00  1.38
ATOM    295  OE2 GLU   344      -2.095   0.607 -14.567  1.00  1.96
ATOM    296  C   GLU   344      -1.418  -0.861  -8.972  1.00  0.42
ATOM    297  O   GLU   344      -1.350  -2.073  -8.911  1.00  0.43
ATOM    298  N   PHE   345      -0.746  -0.096  -8.155  1.00  0.40
ATOM    299  HN  PHE   345      -0.842   0.878  -8.209  1.00  0.40
ATOM    300  CA  PHE   345       0.133  -0.696  -7.117  1.00  0.39
ATOM    301  HA  PHE   345       0.911  -1.281  -7.586  1.00  0.41
ATOM    302  CB  PHE   345       0.754   0.436  -6.287  1.00  0.38
ATOM    303  HB1 PHE   345      -0.028   1.101  -5.953  1.00  0.40
ATOM    304  HB2 PHE   345       1.450   0.987  -6.902  1.00  0.41
ATOM    305  CG  PHE   345       1.485  -0.117  -5.083  1.00  0.36
ATOM    306  CD1 PHE   345       1.435   0.573  -3.867  1.00  1.30
ATOM    307  HD1 PHE   345       0.870   1.491  -3.790  1.00  2.21
ATOM    308  CD2 PHE   345       2.217  -1.306  -5.182  1.00  1.22
```

Figure 8 (5 of 19)

```
ATOM    309  HD2 PHE   345       2.255  -1.842  -6.117  1.00  2.14
ATOM    310  CE1 PHE   345       2.115   0.077  -2.750  1.00  1.31
ATOM    311  HE1 PHE   345       2.075   0.612  -1.812  1.00  2.23
ATOM    312  CE2 PHE   345       2.896  -1.803  -4.064  1.00  1.21
ATOM    313  HE2 PHE   345       3.461  -2.718  -4.141  1.00  2.12
ATOM    314  CZ  PHE   345       2.846  -1.112  -2.848  1.00  0.37
ATOM    315  HZ  PHE   345       3.372  -1.496  -1.986  1.00  0.39
ATOM    316  C   PHE   345      -0.730  -1.594  -6.232  1.00  0.37
ATOM    317  O   PHE   345      -0.282  -2.595  -5.709  1.00  0.37
ATOM    318  N   VAL   346      -1.977  -1.243  -6.083  1.00  0.37
ATOM    319  HN  VAL   346      -2.313  -0.438  -6.529  1.00  0.39
ATOM    320  CA  VAL   346      -2.896  -2.068  -5.259  1.00  0.40
ATOM    321  HA  VAL   346      -2.407  -2.356  -4.339  1.00  0.40
ATOM    322  CB  VAL   346      -4.150  -1.251  -4.944  1.00  0.52
ATOM    323  HB  VAL   346      -4.658  -1.002  -5.865  1.00  1.31
ATOM    324  CG1 VAL   346      -5.084  -2.064  -4.054  1.00  1.22
ATOM    325 HG11 VAL   346      -4.578  -2.309  -3.134  1.00  1.73
ATOM    326 HG12 VAL   346      -5.366  -2.972  -4.565  1.00  1.84
ATOM    327 HG13 VAL   346      -5.968  -1.482  -3.837  1.00  1.77
ATOM    328  CG2 VAL   346      -3.751   0.034  -4.217  1.00  0.88
ATOM    329 HG21 VAL   346      -3.741   0.856  -4.917  1.00  1.44
ATOM    330 HG22 VAL   346      -2.767  -0.085  -3.788  1.00  1.55
ATOM    331 HG23 VAL   346      -4.463   0.240  -3.431  1.00  1.48
ATOM    332  C   VAL   346      -3.276  -3.317  -6.055  1.00  0.37
ATOM    333  O   VAL   346      -3.377  -4.406  -5.519  1.00  0.37
ATOM    334  N   LYS   347      -3.467  -3.171  -7.341  1.00  0.38
ATOM    335  HN  LYS   347      -3.363  -2.289  -7.756  1.00  0.39
ATOM    336  CA  LYS   347      -3.817  -4.351  -8.176  1.00  0.39
ATOM    337  HA  LYS   347      -4.726  -4.803  -7.806  1.00  0.40
ATOM    338  CB  LYS   347      -4.009  -3.915  -9.631  1.00  0.43
ATOM    339  HB1 LYS   347      -3.428  -4.554 -10.278  1.00  0.81
ATOM    340  HB2 LYS   347      -3.681  -2.892  -9.745  1.00  0.77
ATOM    341  CG  LYS   347      -5.489  -4.022 -10.008  1.00  0.92
ATOM    342  HG1 LYS   347      -6.078  -3.422  -9.332  1.00  1.27
ATOM    343  HG2 LYS   347      -5.803  -5.054  -9.942  1.00  1.24
ATOM    344  CD  LYS   347      -5.688  -3.518 -11.440  1.00  1.11
ATOM    345  HD1 LYS   347      -5.098  -4.116 -12.117  1.00  1.38
ATOM    346  HD2 LYS   347      -5.374  -2.486 -11.504  1.00  1.25
ATOM    347  CE  LYS   347      -7.166  -3.628 -11.821  1.00  1.99
ATOM    348  HE1 LYS   347      -7.728  -2.861 -11.309  1.00  2.39
ATOM    349  HE2 LYS   347      -7.540  -4.600 -11.536  1.00  2.52
ATOM    350  NZ  LYS   347      -7.312  -3.451 -13.294  1.00  2.35
ATOM    351  HZ1 LYS   347      -8.189  -2.930 -13.496  1.00  2.93
ATOM    352  HZ2 LYS   347      -7.350  -4.384 -13.753  1.00  2.57
ATOM    353  HZ3 LYS   347      -6.501  -2.915 -13.662  1.00  2.47
ATOM    354  C   LYS   347      -2.671  -5.354  -8.086  1.00  0.39
ATOM    355  O   LYS   347      -2.873  -6.530  -7.854  1.00  0.41
ATOM    356  N   ARG   348      -1.461  -4.890  -8.246  1.00  0.39
ATOM    357  HN  ARG   348      -1.322  -3.935  -8.416  1.00  0.39
ATOM    358  CA  ARG   348      -0.295  -5.806  -8.146  1.00  0.42
ATOM    359  HA  ARG   348      -0.412  -6.624  -8.842  1.00  0.47
ATOM    360  CB  ARG   348       0.990  -5.037  -8.462  1.00  0.45
ATOM    361  HB1 ARG   348       1.843  -5.678  -8.300  1.00  0.75
ATOM    362  HB2 ARG   348       1.061  -4.173  -7.816  1.00  0.95
ATOM    363  CG  ARG   348       0.968  -4.581  -9.923  1.00  1.12
ATOM    364  HG1 ARG   348       1.496  -3.644 -10.016  1.00  1.84
ATOM    365  HG2 ARG   348      -0.055  -4.451 -10.244  1.00  1.77
ATOM    366  CD  ARG   348       1.649  -5.634 -10.799  1.00  1.28
ATOM    367  HD1 ARG   348       1.059  -6.539 -10.797  1.00  1.54
ATOM    368  HD2 ARG   348       2.634  -5.845 -10.409  1.00  1.76
ATOM    369  NE  ARG   348       1.765  -5.120 -12.193  1.00  2.08
ATOM    370  HE  ARG   348       1.642  -4.165 -12.374  1.00  2.58
ATOM    371  CZ  ARG   348       2.032  -5.940 -13.172  1.00  2.53
ATOM    372  NH1 ARG   348       1.143  -6.818 -13.548  1.00  3.15
ATOM    373 HH11 ARG   348       0.257  -6.862 -13.086  1.00  3.43
ATOM    374 HH12 ARG   348       1.347  -7.447 -14.298  1.00  3.63
ATOM    375  NH2 ARG   348       3.188  -5.883 -13.775  1.00  2.91
ATOM    376 HH21 ARG   348       3.869  -5.210 -13.487  1.00  3.03
ATOM    377 HH22 ARG   348       3.392  -6.512 -14.525  1.00  3.41
ATOM    378  C   ARG   348      -0.231  -6.348  -6.719  1.00  0.40
ATOM    379  O   ARG   348       0.253  -7.435  -6.474  1.00  0.43
ATOM    380  N   LEU   349      -0.732  -5.596  -5.774  1.00  0.36
ATOM    381  HN  LEU   349      -1.124  -4.726  -5.997  1.00  0.35
ATOM    382  CA  LEU   349      -0.718  -6.060  -4.360  1.00  0.37
ATOM    383  HA  LEU   349       0.302  -6.157  -4.020  1.00  0.39
ATOM    384  CB  LEU   349      -1.454  -5.043  -3.486  1.00  0.36
ATOM    385  HB1 LEU   349      -2.389  -5.464  -3.149  1.00  0.48
```

```
ATOM    386  HB2 LEU   349      -1.649  -4.149  -4.062  1.00  0.41
ATOM    387  CG  LEU   349      -0.589  -4.692  -2.275  1.00  0.40
ATOM    388  HG  LEU   349       0.051  -5.529  -2.036  1.00  0.65
ATOM    389  CD1 LEU   349       0.270  -3.469  -2.600  1.00  0.52
ATOM    390 HD11 LEU   349       1.268  -3.789  -2.859  1.00  1.02
ATOM    391 HD12 LEU   349       0.313  -2.820  -1.737  1.00  1.18
ATOM    392 HD13 LEU   349      -0.165  -2.934  -3.431  1.00  1.30
ATOM    393  CD2 LEU   349      -1.491  -4.378  -1.081  1.00  0.56
ATOM    394 HD21 LEU   349      -1.483  -3.315  -0.894  1.00  1.15
ATOM    395 HD22 LEU   349      -1.127  -4.901  -0.208  1.00  1.15
ATOM    396 HD23 LEU   349      -2.500  -4.698  -1.298  1.00  1.11
ATOM    397  C   LEU   349      -1.417  -7.418  -4.274  1.00  0.38
ATOM    398  O   LEU   349      -0.853  -8.389  -3.811  1.00  0.40
ATOM    399  N   GLY   350      -2.637  -7.499  -4.731  1.00  0.38
ATOM    400  HN  GLY   350      -3.073  -6.706  -5.113  1.00  0.39
ATOM    401  CA  GLY   350      -3.358  -8.804  -4.686  1.00  0.41
ATOM    402  HA1 GLY   350      -2.725  -9.545  -4.220  1.00  0.49
ATOM    403  HA2 GLY   350      -3.593  -9.117  -5.693  1.00  0.46
ATOM    404  C   GLY   350      -4.653  -8.672  -3.880  1.00  0.32
ATOM    405  O   GLY   350      -5.238  -9.655  -3.471  1.00  0.32
ATOM    406  N   LEU   351      -5.114  -7.473  -3.650  1.00  0.31
ATOM    407  HN  LEU   351      -4.637  -6.688  -3.988  1.00  0.35
ATOM    408  CA  LEU   351      -6.375  -7.304  -2.876  1.00  0.28
ATOM    409  HA  LEU   351      -6.460  -8.100  -2.151  1.00  0.31
ATOM    410  CB  LEU   351      -6.359  -5.956  -2.153  1.00  0.34
ATOM    411  HB1 LEU   351      -6.954  -5.244  -2.705  1.00  0.78
ATOM    412  HB2 LEU   351      -5.342  -5.598  -2.082  1.00  0.74
ATOM    413  CG  LEU   351      -6.943  -6.124  -0.749  1.00  0.69
ATOM    414  HG  LEU   351      -7.915  -6.590  -0.818  1.00  1.53
ATOM    415  CD1 LEU   351      -6.014  -7.004   0.090  1.00  1.03
ATOM    416 HD11 LEU   351      -5.298  -7.491  -0.556  1.00  1.65
ATOM    417 HD12 LEU   351      -6.598  -7.751   0.608  1.00  1.55
ATOM    418 HD13 LEU   351      -5.492  -6.393   0.811  1.00  1.45
ATOM    419  CD2 LEU   351      -7.078  -4.751  -0.087  1.00  1.36
ATOM    420 HD21 LEU   351      -7.424  -4.034  -0.816  1.00  1.71
ATOM    421 HD22 LEU   351      -6.118  -4.440   0.297  1.00  1.92
ATOM    422 HD23 LEU   351      -7.788  -4.811   0.724  1.00  1.96
ATOM    423  C   LEU   351      -7.566  -7.358  -3.833  1.00  0.28
ATOM    424  O   LEU   351      -7.434  -7.119  -5.017  1.00  0.30
ATOM    425  N   SER   352      -8.730  -7.674  -3.333  1.00  0.32
ATOM    426  HN  SER   352      -8.815  -7.866  -2.376  1.00  0.35
ATOM    427  CA  SER   352      -9.928  -7.746  -4.218  1.00  0.39
ATOM    428  HA  SER   352      -9.812  -8.564  -4.914  1.00  0.42
ATOM    429  CB  SER   352     -11.176  -7.977  -3.366  1.00  0.50
ATOM    430  HB1 SER   352     -11.572  -7.022  -3.044  1.00  0.91
ATOM    431  HB2 SER   352     -10.921  -8.566  -2.501  1.00  0.98
ATOM    432  OG  SER   352     -12.147  -8.672  -4.136  1.00  1.21
ATOM    433  HG  SER   352     -12.309  -9.520  -3.715  1.00  1.44
ATOM    434  C   SER   352     -10.076  -6.435  -4.993  1.00  0.38
ATOM    435  O   SER   352     -10.150  -5.367  -4.418  1.00  0.36
ATOM    436  N   ASP   353     -10.120  -6.507  -6.296  1.00  0.41
ATOM    437  HN  ASP   353     -10.060  -7.379  -6.740  1.00  0.44
ATOM    438  CA  ASP   353     -10.265  -5.266  -7.108  1.00  0.42
ATOM    439  HA  ASP   353      -9.387  -4.650  -6.984  1.00  0.41
ATOM    440  CB  ASP   353     -10.422  -5.639  -8.584  1.00  0.49
ATOM    441  HB1 ASP   353     -11.358  -5.249  -8.956  1.00  1.06
ATOM    442  HB2 ASP   353     -10.413  -6.714  -8.686  1.00  1.01
ATOM    443  CG  ASP   353      -9.267  -5.039  -9.388  1.00  1.39
ATOM    444  OD1 ASP   353      -9.539  -4.389 -10.384  1.00  2.17
ATOM    445  OD2 ASP   353      -8.130  -5.241  -8.995  1.00  2.10
ATOM    446  C   ASP   353     -11.501  -4.493  -6.643  1.00  0.43
ATOM    447  O   ASP   353     -11.497  -3.280  -6.574  1.00  0.40
ATOM    448  N   HIS   354     -12.558  -5.187  -6.319  1.00  0.50
ATOM    449  HN  HIS   354     -12.540  -6.165  -6.379  1.00  0.55
ATOM    450  CA  HIS   354     -13.790  -4.490  -5.856  1.00  0.56
ATOM    451  HA  HIS   354     -14.088  -3.757  -6.591  1.00  0.58
ATOM    452  CB  HIS   354     -14.914  -5.511  -5.663  1.00  0.68
ATOM    453  HB1 HIS   354     -15.268  -5.468  -4.644  1.00  1.10
ATOM    454  HB2 HIS   354     -14.539  -6.502  -5.873  1.00  1.33
ATOM    455  CG  HIS   354     -16.047  -5.194  -6.600  1.00  1.29
ATOM    456  ND1 HIS   354     -15.862  -5.075  -7.969  1.00  2.24
ATOM    457  HD1 HIS   354     -15.015  -5.182  -8.450  1.00  2.68
ATOM    458  CD2 HIS   354     -17.382  -4.965  -6.381  1.00  2.16
ATOM    459  HD2 HIS   354     -17.866  -4.981  -5.416  1.00  2.62
ATOM    460  CE1 HIS   354     -17.057  -4.787  -8.516  1.00  3.03
ATOM    461  HE1 HIS   354     -17.219  -4.638  -9.573  1.00  3.92
ATOM    462  NE2 HIS   354     -18.019  -4.708  -7.592  1.00  3.02
```

```
ATOM    463  C    HIS   354      -13.502   -3.790   -4.528   1.00   0.49
ATOM    464  O    HIS   354      -13.852   -2.643   -4.332   1.00   0.49
ATOM    465  N    GLU   355      -12.860   -4.467   -3.616   1.00   0.49
ATOM    466  HN   GLU   355      -12.581   -5.389   -3.794   1.00   0.50
ATOM    467  CA   GLU   355      -12.546   -3.832   -2.306   1.00   0.49
ATOM    468  HA   GLU   355      -13.465   -3.596   -1.789   1.00   0.56
ATOM    469  CB   GLU   355      -11.713   -4.794   -1.456   1.00   0.55
ATOM    470  HB1  GLU   355      -10.802   -5.041   -1.980   1.00   0.96
ATOM    471  HB2  GLU   355      -12.280   -5.695   -1.273   1.00   0.95
ATOM    472  CG   GLU   355      -11.366   -4.128   -0.123   1.00   1.01
ATOM    473  HG1  GLU   355      -12.239   -3.628    0.267   1.00   1.63
ATOM    474  HG2  GLU   355      -10.575   -3.408   -0.276   1.00   1.68
ATOM    475  CD   GLU   355      -10.904   -5.192    0.873   1.00   1.40
ATOM    476  OE1  GLU   355       -9.849   -5.010    1.458   1.00   2.07
ATOM    477  OE2  GLU   355      -11.613   -6.172    1.033   1.00   1.91
ATOM    478  C    GLU   355      -11.753   -2.548   -2.551   1.00   0.40
ATOM    479  O    GLU   355      -11.879   -1.581   -1.828   1.00   0.43
ATOM    480  N    ILE   356      -10.942   -2.533   -3.574   1.00   0.33
ATOM    481  HN   ILE   356      -10.861   -3.324   -4.146   1.00   0.34
ATOM    482  CA   ILE   356      -10.143   -1.313   -3.876   1.00   0.30
ATOM    483  HA   ILE   356       -9.520   -1.071   -3.028   1.00   0.35
ATOM    484  CB   ILE   356       -9.258   -1.577   -5.097   1.00   0.33
ATOM    485  HB   ILE   356       -9.875   -1.872   -5.933   1.00   0.36
ATOM    486  CG1  ILE   356       -8.270   -2.698   -4.766   1.00   0.39
ATOM    487  HG11 ILE   356       -8.815   -3.601   -4.537   1.00   0.38
ATOM    488  HG12 ILE   356       -7.674   -2.411   -3.913   1.00   0.43
ATOM    489  CG2  ILE   356       -8.484   -0.305   -5.457   1.00   0.39
ATOM    490  HG21 ILE   356       -8.663    0.450   -4.706   1.00   1.08
ATOM    491  HG22 ILE   356       -8.816    0.057   -6.419   1.00   1.06
ATOM    492  HG23 ILE   356       -7.428   -0.527   -5.501   1.00   1.06
ATOM    493  CD1  ILE   356       -7.357   -2.947   -5.967   1.00   0.47
ATOM    494  HD11 ILE   356       -6.572   -2.207   -5.981   1.00   1.16
ATOM    495  HD12 ILE   356       -7.934   -2.878   -6.877   1.00   1.16
ATOM    496  HD13 ILE   356       -6.922   -3.933   -5.889   1.00   1.07
ATOM    497  C    ILE   356      -11.090   -0.147   -4.167   1.00   0.31
ATOM    498  O    ILE   356      -10.833    0.981   -3.799   1.00   0.34
ATOM    499  N    ASP   357      -12.187   -0.412   -4.824   1.00   0.34
ATOM    500  HN   ASP   357      -12.378   -1.330   -5.111   1.00   0.37
ATOM    501  CA   ASP   357      -13.151    0.681   -5.134   1.00   0.40
ATOM    502  HA   ASP   357      -12.619    1.522   -5.554   1.00   0.43
ATOM    503  CB   ASP   357      -14.187    0.178   -6.142   1.00   0.48
ATOM    504  HB1  ASP   357      -15.158    0.575   -5.888   1.00   0.96
ATOM    505  HB2  ASP   357      -14.220   -0.901   -6.115   1.00   0.95
ATOM    506  CG   ASP   357      -13.801    0.642   -7.548   1.00   1.24
ATOM    507  OD1  ASP   357      -13.679   -0.205   -8.417   1.00   1.82
ATOM    508  OD2  ASP   357      -13.635    1.837   -7.732   1.00   2.06
ATOM    509  C    ASP   357      -13.858    1.113   -3.848   1.00   0.41
ATOM    510  O    ASP   357      -14.333    2.226   -3.733   1.00   0.45
ATOM    511  N    ARG   358      -13.932    0.241   -2.880   1.00   0.43
ATOM    512  HN   ARG   358      -13.543   -0.651   -2.995   1.00   0.44
ATOM    513  CA   ARG   358      -14.609    0.599   -1.601   1.00   0.49
ATOM    514  HA   ARG   358      -15.482    1.186   -1.816   1.00   0.50
ATOM    515  CB   ARG   358      -15.019   -0.677   -0.863   1.00   0.57
ATOM    516  HB1  ARG   358      -15.605   -0.417    0.006   1.00   0.92
ATOM    517  HB2  ARG   358      -14.134   -1.214   -0.554   1.00   0.75
ATOM    518  CG   ARG   358      -15.854   -1.561   -1.791   1.00   1.10
ATOM    519  HG1  ARG   358      -15.244   -1.895   -2.616   1.00   1.46
ATOM    520  HG2  ARG   358      -16.693   -0.995   -2.168   1.00   1.66
ATOM    521  CD   ARG   358      -16.365   -2.777   -1.015   1.00   1.30
ATOM    522  HD1  ARG   358      -15.551   -3.214   -0.455   1.00   1.75
ATOM    523  HD2  ARG   358      -16.759   -3.506   -1.707   1.00   1.56
ATOM    524  NE   ARG   358      -17.441   -2.352   -0.076   1.00   1.98
ATOM    525  HE   ARG   358      -17.515   -1.412    0.193   1.00   2.56
ATOM    526  CZ   ARG   358      -18.286   -3.232    0.390   1.00   2.40
ATOM    527  NH1  ARG   358      -18.371   -3.438    1.676   1.00   3.04
ATOM    528  HH11 ARG   358      -17.790   -2.922    2.305   1.00   3.32
ATOM    529  HH12 ARG   358      -19.018   -4.112    2.032   1.00   3.55
ATOM    530  NH2  ARG   358      -19.044   -3.905   -0.431   1.00   2.82
ATOM    531  HH21 ARG   358      -18.979   -3.747   -1.416   1.00   3.00
ATOM    532  HH22 ARG   358      -19.691   -4.579   -0.075   1.00   3.31
ATOM    533  C    ARG   358      -13.660    1.412   -0.720   1.00   0.50
ATOM    534  O    ARG   358      -14.079    2.100    0.190   1.00   0.56
ATOM    535  N    LEU   359      -12.388    1.337   -0.979   1.00   0.48
ATOM    536  HN   LEU   359      -12.077    0.777   -1.715   1.00   0.45
ATOM    537  CA   LEU   359      -11.412    2.104   -0.151   1.00   0.54
ATOM    538  HA   LEU   359      -11.525    1.824    0.886   1.00   0.61
ATOM    539  CB   LEU   359       -9.978    1.800   -0.608   1.00   0.56
```

```
ATOM    540  HB1 LEU   359      -9.284   2.152   0.141  1.00  0.78
ATOM    541  HB2 LEU   359      -9.786   2.309  -1.541  1.00  0.86
ATOM    542  CG  LEU   359      -9.784   0.291  -0.806  1.00  0.58
ATOM    543  HG  LEU   359     -10.359  -0.035  -1.658  1.00  1.08
ATOM    544  CD1 LEU   359      -8.304  -0.003  -1.054  1.00  0.81
ATOM    545 HD11 LEU   359      -7.991   0.471  -1.972  1.00  1.55
ATOM    546 HD12 LEU   359      -8.157  -1.070  -1.131  1.00  1.29
ATOM    547 HD13 LEU   359      -7.719   0.382  -0.232  1.00  1.26
ATOM    548  CD2 LEU   359     -10.240  -0.469   0.443  1.00  0.98
ATOM    549 HD21 LEU   359     -11.287  -0.717   0.351  1.00  1.62
ATOM    550 HD22 LEU   359     -10.091   0.150   1.315  1.00  1.46
ATOM    551 HD23 LEU   359      -9.662  -1.376   0.542  1.00  1.49
ATOM    552  C   LEU   359     -11.684   3.601  -0.305  1.00  0.58
ATOM    553  O   LEU   359     -11.683   4.343   0.657  1.00  0.67
ATOM    554  N   GLU   360     -11.916   4.050  -1.507  1.00  0.59
ATOM    555  HN  GLU   360     -11.913   3.435  -2.270  1.00  0.56
ATOM    556  CA  GLU   360     -12.188   5.499  -1.720  1.00  0.72
ATOM    557  HA  GLU   360     -11.354   6.079  -1.352  1.00  0.78
ATOM    558  CB  GLU   360     -12.379   5.770  -3.213  1.00  0.81
ATOM    559  HB1 GLU   360     -13.419   5.640  -3.473  1.00  1.05
ATOM    560  HB2 GLU   360     -11.775   5.080  -3.784  1.00  0.96
ATOM    561  CG  GLU   360     -11.953   7.205  -3.530  1.00  1.67
ATOM    562  HG1 GLU   360     -11.009   7.414  -3.050  1.00  2.26
ATOM    563  HG2 GLU   360     -12.703   7.892  -3.164  1.00  2.21
ATOM    564  CD  GLU   360     -11.802   7.371  -5.043  1.00  1.94
ATOM    565  OE1 GLU   360     -12.814   7.358  -5.724  1.00  2.33
ATOM    566  OE2 GLU   360     -10.677   7.508  -5.494  1.00  2.49
ATOM    567  C   GLU   360     -13.456   5.894  -0.962  1.00  0.76
ATOM    568  O   GLU   360     -13.577   6.997  -0.466  1.00  0.86
ATOM    569  N   LEU   361     -14.403   5.001  -0.868  1.00  0.74
ATOM    570  HN  LEU   361     -14.285   4.117  -1.274  1.00  0.69
ATOM    571  CA  LEU   361     -15.662   5.325  -0.141  1.00  0.86
ATOM    572  HA  LEU   361     -16.056   6.264  -0.503  1.00  0.95
ATOM    573  CB  LEU   361     -16.688   4.215  -0.382  1.00  0.96
ATOM    574  HB1 LEU   361     -16.739   3.577   0.488  1.00  1.36
ATOM    575  HB2 LEU   361     -16.391   3.631  -1.241  1.00  1.11
ATOM    576  CG  LEU   361     -18.063   4.834  -0.636  1.00  1.71
ATOM    577  HG  LEU   361     -18.061   5.863  -0.306  1.00  2.43
ATOM    578  CD1 LEU   361     -18.381   4.780  -2.131  1.00  2.03
ATOM    579 HD11 LEU   361     -17.459   4.767  -2.695  1.00  2.51
ATOM    580 HD12 LEU   361     -18.959   5.649  -2.408  1.00  2.43
ATOM    581 HD13 LEU   361     -18.948   3.887  -2.347  1.00  2.25
ATOM    582  CD2 LEU   361     -19.125   4.050   0.137  1.00  2.33
ATOM    583 HD21 LEU   361     -18.693   3.135   0.515  1.00  2.74
ATOM    584 HD22 LEU   361     -19.949   3.814  -0.520  1.00  2.84
ATOM    585 HD23 LEU   361     -19.484   4.646   0.963  1.00  2.65
ATOM    586  C   LEU   361     -15.371   5.437   1.357  1.00  0.89
ATOM    587  O   LEU   361     -15.986   6.211   2.063  1.00  1.03
ATOM    588  N   GLN   362     -14.435   4.669   1.848  1.00  0.83
ATOM    589  HN  GLN   362     -13.950   4.052   1.261  1.00  0.76
ATOM    590  CA  GLN   362     -14.104   4.732   3.300  1.00  0.95
ATOM    591  HA  GLN   362     -14.952   4.394   3.877  1.00  1.11
ATOM    592  CB  GLN   362     -12.900   3.834   3.589  1.00  0.97
ATOM    593  HB1 GLN   362     -12.015   4.442   3.701  1.00  1.37
ATOM    594  HB2 GLN   362     -12.761   3.143   2.769  1.00  1.26
ATOM    595  CG  GLN   362     -13.144   3.051   4.881  1.00  1.37
ATOM    596  HG1 GLN   362     -14.040   2.459   4.779  1.00  1.85
ATOM    597  HG2 GLN   362     -13.260   3.743   5.703  1.00  2.00
ATOM    598  CD  GLN   362     -11.954   2.129   5.153  1.00  1.42
ATOM    599  OE1 GLN   362     -10.989   2.129   4.415  1.00  1.39
ATOM    600  NE2 GLN   362     -11.983   1.336   6.190  1.00  2.20
ATOM    601 HE21 GLN   362     -12.761   1.336   6.785  1.00  2.72
ATOM    602 HE22 GLN   362     -11.226   0.742   6.373  1.00  2.46
ATOM    603  C   GLN   362     -13.768   6.174   3.686  1.00  1.04
ATOM    604  O   GLN   362     -14.293   6.709   4.642  1.00  1.30
ATOM    605  N   ASN   363     -12.896   6.809   2.950  1.00  1.02
ATOM    606  HN  ASN   363     -12.483   6.360   2.183  1.00  1.03
ATOM    607  CA  ASN   363     -12.529   8.214   3.279  1.00  1.24
ATOM    608  HA  ASN   363     -13.404   8.741   3.631  1.00  1.45
ATOM    609  CB  ASN   363     -11.459   8.218   4.373  1.00  1.35
ATOM    610  HB1 ASN   363     -10.738   8.994   4.170  1.00  1.46
ATOM    611  HB2 ASN   363     -10.962   7.259   4.392  1.00  1.49
ATOM    612  CG  ASN   363     -12.118   8.479   5.728  1.00  2.07
ATOM    613  OD1 ASN   363     -12.924   9.378   5.862  1.00  2.60
ATOM    614  ND2 ASN   363     -11.809   7.724   6.747  1.00  2.76
ATOM    615 HD21 ASN   363     -11.159   6.999   6.640  1.00  2.99
ATOM    616 HD22 ASN   363     -12.227   7.883   7.619  1.00  3.34
```

```
ATOM    617  C    ASN   363      -11.987   8.908   2.028  1.00  1.40
ATOM    618  O    ASN   363      -10.813   9.206   1.930  1.00  2.25
ATOM    619  N    GLY   364      -12.834   9.166   1.069  1.00  1.09
ATOM    620  HN   GLY   364      -13.777   8.917   1.169  1.00  1.35
ATOM    621  CA   GLY   364      -12.371   9.840  -0.177  1.00  1.25
ATOM    622  HA1  GLY   364      -13.191   9.907  -0.876  1.00  1.54
ATOM    623  HA2  GLY   364      -11.569   9.264  -0.618  1.00  1.26
ATOM    624  C    GLY   364      -11.868  11.249   0.148  1.00  1.27
ATOM    625  O    GLY   364      -11.155  11.856  -0.626  1.00  1.55
ATOM    626  N    ARG   365      -12.234  11.780   1.286  1.00  1.27
ATOM    627  HN   ARG   365      -12.811  11.278   1.898  1.00  1.42
ATOM    628  CA   ARG   365      -11.777  13.151   1.654  1.00  1.36
ATOM    629  HA   ARG   365      -12.239  13.872   0.997  1.00  1.70
ATOM    630  CB   ARG   365      -12.178  13.450   3.100  1.00  1.65
ATOM    631  HB1  ARG   365      -11.321  13.822   3.641  1.00  1.87
ATOM    632  HB2  ARG   365      -12.535  12.544   3.568  1.00  2.13
ATOM    633  CG   ARG   365      -13.286  14.506   3.116  1.00  2.23
ATOM    634  HG1  ARG   365      -13.961  14.332   2.291  1.00  2.71
ATOM    635  HG2  ARG   365      -12.848  15.489   3.021  1.00  2.50
ATOM    636  CD   ARG   365      -14.059  14.415   4.433  1.00  2.72
ATOM    637  HD1  ARG   365      -14.622  13.494   4.458  1.00  2.80
ATOM    638  HD2  ARG   365      -14.737  15.253   4.510  1.00  3.17
ATOM    639  NE   ARG   365      -13.102  14.445   5.574  1.00  3.34
ATOM    640  HE   ARG   365      -12.202  14.073   5.468  1.00  3.67
ATOM    641  CZ   ARG   365      -13.463  14.966   6.714  1.00  3.90
ATOM    642  NH1  ARG   365      -12.721  15.879   7.279  1.00  4.42
ATOM    643  HH11 ARG   365      -11.875  16.179   6.838  1.00  4.48
ATOM    644  HH12 ARG   365      -12.998  16.279   8.153  1.00  4.97
ATOM    645  NH2  ARG   365      -14.567  14.575   7.290  1.00  4.33
ATOM    646  HH21 ARG   365      -15.136  13.876   6.857  1.00  4.29
ATOM    647  HH22 ARG   365      -14.844  14.975   8.164  1.00  4.93
ATOM    648  C    ARG   365      -10.254  13.242   1.518  1.00  0.94
ATOM    649  O    ARG   365       -9.739  13.797   0.567  1.00  1.24
ATOM    650  N    CYS   366       -9.529  12.701   2.459  1.00  0.68
ATOM    651  HN   CYS   366       -9.962  12.257   3.217  1.00  0.91
ATOM    652  CA   CYS   366       -8.043  12.759   2.378  1.00  0.77
ATOM    653  HA   CYS   366       -7.745  13.675   1.890  1.00  1.02
ATOM    654  CB   CYS   366       -7.450  12.716   3.787  1.00  1.12
ATOM    655  HB1  CYS   366       -6.580  12.076   3.793  1.00  1.32
ATOM    656  HB2  CYS   366       -8.186  12.329   4.476  1.00  1.41
ATOM    657  SG   CYS   366       -6.972  14.387   4.291  1.00  1.97
ATOM    658  HG   CYS   366       -7.177  14.985   3.568  1.00  2.29
ATOM    659  C    CYS   366       -7.530  11.564   1.572  1.00  0.67
ATOM    660  O    CYS   366       -7.880  10.430   1.833  1.00  0.66
ATOM    661  N    LEU   367       -6.705  11.809   0.592  1.00  0.68
ATOM    662  HN   LEU   367       -6.437  12.731   0.397  1.00  0.77
ATOM    663  CA   LEU   367       -6.172  10.689  -0.232  1.00  0.65
ATOM    664  HA   LEU   367       -6.992  10.170  -0.707  1.00  0.65
ATOM    665  CB   LEU   367       -5.235  11.247  -1.303  1.00  0.79
ATOM    666  HB1  LEU   367       -4.373  11.692  -0.831  1.00  1.21
ATOM    667  HB2  LEU   367       -5.757  11.995  -1.883  1.00  1.27
ATOM    668  CG   LEU   367       -4.782  10.113  -2.222  1.00  1.20
ATOM    669  HG   LEU   367       -4.447   9.278  -1.624  1.00  1.65
ATOM    670  CD1  LEU   367       -5.951   9.673  -3.105  1.00  1.87
ATOM    671  HD11 LEU   367       -6.575  10.525  -3.327  1.00  2.32
ATOM    672  HD12 LEU   367       -6.533   8.926  -2.585  1.00  2.43
ATOM    673  HD13 LEU   367       -5.570   9.256  -4.025  1.00  2.19
ATOM    674  CD2  LEU   367       -3.634  10.606  -3.103  1.00  1.50
ATOM    675  HD21 LEU   367       -3.857  10.392  -4.138  1.00  1.88
ATOM    676  HD22 LEU   367       -2.722  10.104  -2.819  1.00  1.84
ATOM    677  HD23 LEU   367       -3.513  11.672  -2.974  1.00  2.01
ATOM    678  C    LEU   367       -5.403   9.715   0.663  1.00  0.56
ATOM    679  O    LEU   367       -5.581   8.515   0.586  1.00  0.53
ATOM    680  N    ARG   368       -4.551  10.220   1.516  1.00  0.56
ATOM    681  HN   ARG   368       -4.425  11.191   1.564  1.00  0.62
ATOM    682  CA   ARG   368       -3.772   9.323   2.422  1.00  0.51
ATOM    683  HA   ARG   368       -3.041   8.768   1.846  1.00  0.50
ATOM    684  CB   ARG   368       -3.053  10.167   3.477  1.00  0.58
ATOM    685  HB1  ARG   368       -3.231   9.746   4.456  1.00  1.21
ATOM    686  HB2  ARG   368       -3.431  11.179   3.446  1.00  0.95
ATOM    687  CG   ARG   368       -1.550  10.173   3.193  1.00  1.39
ATOM    688  HG1  ARG   368       -1.368  10.626   2.230  1.00  1.89
ATOM    689  HG2  ARG   368       -1.180   9.158   3.190  1.00  2.10
ATOM    690  CD   ARG   368       -0.830  10.978   4.276  1.00  1.56
ATOM    691  HD1  ARG   368        0.130  10.529   4.480  1.00  2.12
ATOM    692  HD2  ARG   368       -1.425  10.981   5.177  1.00  1.61
ATOM    693  NE   ARG   368       -0.634  12.378   3.804  1.00  2.27
```

Figure 8 (10 of 19)

```
ATOM    694  HE  ARG   368       -1.079  12.686   2.987  1.00  2.72
ATOM    695  CZ  ARG   368        0.130  13.193   4.478  1.00  2.82
ATOM    696  NH1 ARG   368        0.010  13.279   5.775  1.00  3.23
ATOM    697 HH11 ARG   368       -0.668  12.720   6.253  1.00  3.31
ATOM    698 HH12 ARG   368        0.596  13.904   6.291  1.00  3.77
ATOM    699  NH2 ARG   368        1.014  13.923   3.854  1.00  3.43
ATOM    700 HH21 ARG   368        1.105  13.858   2.861  1.00  3.61
ATOM    701 HH22 ARG   368        1.600  14.548   4.370  1.00  3.97
ATOM    702  C   ARG   368       -4.721   8.343   3.116  1.00  0.47
ATOM    703  O   ARG   368       -4.368   7.218   3.391  1.00  0.42
ATOM    704  N   GLU   369       -5.926   8.758   3.395  1.00  0.51
ATOM    705  HN  GLU   369       -6.199   9.669   3.160  1.00  0.55
ATOM    706  CA  GLU   369       -6.886   7.839   4.065  1.00  0.51
ATOM    707  HA  GLU   369       -6.457   7.486   4.991  1.00  0.52
ATOM    708  CB  GLU   369       -8.193   8.580   4.354  1.00  0.59
ATOM    709  HB1 GLU   369       -8.985   8.162   3.751  1.00  0.79
ATOM    710  HB2 GLU   369       -8.073   9.628   4.117  1.00  1.16
ATOM    711  CG  GLU   369       -8.549   8.428   5.834  1.00  1.21
ATOM    712  HG1 GLU   369       -7.644   8.399   6.421  1.00  1.98
ATOM    713  HG2 GLU   369       -9.102   7.511   5.978  1.00  1.67
ATOM    714  CD  GLU   369       -9.404   9.616   6.280  1.00  1.53
ATOM    715  OE1 GLU   369      -10.074   9.492   7.292  1.00  2.22
ATOM    716  OE2 GLU   369       -9.375  10.630   5.602  1.00  1.87
ATOM    717  C   GLU   369       -7.163   6.648   3.150  1.00  0.49
ATOM    718  O   GLU   369       -7.149   5.510   3.575  1.00  0.50
ATOM    719  N   ALA   370       -7.404   6.898   1.893  1.00  0.50
ATOM    720  HN  ALA   370       -7.403   7.823   1.568  1.00  0.51
ATOM    721  CA  ALA   370       -7.670   5.776   0.953  1.00  0.52
ATOM    722  HA  ALA   370       -8.472   5.163   1.337  1.00  0.55
ATOM    723  CB  ALA   370       -8.059   6.334  -0.417  1.00  0.59
ATOM    724  HB1 ALA   370       -7.938   7.407  -0.415  1.00  1.16
ATOM    725  HB2 ALA   370       -9.090   6.089  -0.626  1.00  1.02
ATOM    726  HB3 ALA   370       -7.425   5.901  -1.176  1.00  1.17
ATOM    727  C   ALA   370       -6.402   4.933   0.820  1.00  0.46
ATOM    728  O   ALA   370       -6.425   3.727   0.969  1.00  0.44
ATOM    729  N   GLN   371       -5.291   5.562   0.551  1.00  0.45
ATOM    730  HN  GLN   371       -5.292   6.536   0.442  1.00  0.48
ATOM    731  CA  GLN   371       -4.021   4.799   0.421  1.00  0.41
ATOM    732  HA  GLN   371       -4.127   4.049  -0.352  1.00  0.42
ATOM    733  CB  GLN   371       -2.880   5.754   0.061  1.00  0.45
ATOM    734  HB1 GLN   371       -2.031   5.185  -0.287  1.00  0.89
ATOM    735  HB2 GLN   371       -2.598   6.324   0.935  1.00  0.83
ATOM    736  CG  GLN   371       -3.336   6.709  -1.045  1.00  0.79
ATOM    737  HG1 GLN   371       -3.604   7.661  -0.611  1.00  1.41
ATOM    738  HG2 GLN   371       -4.194   6.289  -1.551  1.00  1.47
ATOM    739  CD  GLN   371       -2.199   6.910  -2.048  1.00  1.42
ATOM    740  OE1 GLN   371       -2.220   6.354  -3.128  1.00  2.12
ATOM    741  NE2 GLN   371       -1.199   7.688  -1.735  1.00  2.08
ATOM    742 HE21 GLN   371       -1.181   8.138  -0.865  1.00  2.32
ATOM    743 HE22 GLN   371       -0.464   7.821  -2.370  1.00  2.71
ATOM    744  C   GLN   371       -3.718   4.117   1.755  1.00  0.37
ATOM    745  O   GLN   371       -3.287   2.982   1.798  1.00  0.35
ATOM    746  N   TYR   372       -3.955   4.794   2.849  1.00  0.38
ATOM    747  HN  TYR   372       -4.315   5.705   2.798  1.00  0.41
ATOM    748  CA  TYR   372       -3.693   4.167   4.172  1.00  0.38
ATOM    749  HA  TYR   372       -2.712   3.713   4.167  1.00  0.37
ATOM    750  CB  TYR   372       -3.766   5.221   5.278  1.00  0.43
ATOM    751  HB1 TYR   372       -4.797   5.391   5.549  1.00  0.46
ATOM    752  HB2 TYR   372       -3.326   6.142   4.929  1.00  0.45
ATOM    753  CG  TYR   372       -3.004   4.730   6.483  1.00  0.43
ATOM    754  CD1 TYR   372       -3.630   3.899   7.420  1.00  1.25
ATOM    755  HD1 TYR   372       -4.662   3.611   7.282  1.00  2.15
ATOM    756  CD2 TYR   372       -1.667   5.103   6.661  1.00  1.32
ATOM    757  HD2 TYR   372       -1.185   5.744   5.938  1.00  2.21
ATOM    758  CE1 TYR   372       -2.918   3.442   8.535  1.00  1.26
ATOM    759  HE1 TYR   372       -3.400   2.800   9.258  1.00  2.15
ATOM    760  CE2 TYR   372       -0.955   4.647   7.776  1.00  1.34
ATOM    761  HE2 TYR   372        0.077   4.935   7.912  1.00  2.24
ATOM    762  CZ  TYR   372       -1.580   3.816   8.713  1.00  0.51
ATOM    763  OH  TYR   372       -0.878   3.366   9.812  1.00  0.57
ATOM    764  HH  TYR   372       -1.260   3.771  10.594  1.00  0.96
ATOM    765  C   TYR   372       -4.749   3.094   4.416  1.00  0.38
ATOM    766  O   TYR   372       -4.512   2.119   5.100  1.00  0.39
ATOM    767  N   SER   373       -5.913   3.260   3.848  1.00  0.40
ATOM    768  HN  SER   373       -6.079   4.049   3.290  1.00  0.42
ATOM    769  CA  SER   373       -6.978   2.240   4.033  1.00  0.43
ATOM    770  HA  SER   373       -7.177   2.110   5.087  1.00  0.45
```

Figure 8 (11 of 19)

```
ATOM    771  CB  SER   373       -8.253   2.689   3.317  1.00  0.48
ATOM    772  HB1 SER   373       -8.878   1.828   3.123  1.00  1.00
ATOM    773  HB2 SER   373       -7.997   3.162   2.384  1.00  0.75
ATOM    774  OG  SER   373       -8.948   3.619   4.138  1.00  1.18
ATOM    775  HG  SER   373       -9.193   4.371   3.592  1.00  1.47
ATOM    776  C   SER   373       -6.490   0.921   3.437  1.00  0.41
ATOM    777  O   SER   373       -6.780  -0.145   3.937  1.00  0.44
ATOM    778  N   MET   374       -5.732   0.992   2.377  1.00  0.38
ATOM    779  HN  MET   374       -5.502   1.867   1.999  1.00  0.38
ATOM    780  CA  MET   374       -5.200  -0.249   1.749  1.00  0.36
ATOM    781  HA  MET   374       -5.998  -0.967   1.632  1.00  0.39
ATOM    782  CB  MET   374       -4.614   0.110   0.365  1.00  0.36
ATOM    783  HB1 MET   374       -4.139   1.078   0.424  1.00  0.38
ATOM    784  HB2 MET   374       -5.416   0.155  -0.356  1.00  0.40
ATOM    785  CG  MET   374       -3.580  -0.932  -0.098  1.00  0.35
ATOM    786  HG1 MET   374       -2.719  -0.894   0.553  1.00  0.76
ATOM    787  HG2 MET   374       -3.274  -0.708  -1.109  1.00  0.77
ATOM    788  SD  MET   374       -4.304  -2.589  -0.043  1.00  1.06
ATOM    789  CE  MET   374       -5.776  -2.214  -1.020  1.00  0.38
ATOM    790  HE1 MET   374       -5.989  -3.043  -1.679  1.00  1.01
ATOM    791  HE2 MET   374       -5.602  -1.326  -1.606  1.00  1.16
ATOM    792  HE3 MET   374       -6.613  -2.048  -0.356  1.00  1.05
ATOM    793  C   MET   374       -4.116  -0.828   2.666  1.00  0.33
ATOM    794  O   MET   374       -4.136  -1.991   3.018  1.00  0.37
ATOM    795  N   LEU   375       -3.173  -0.017   3.048  1.00  0.31
ATOM    796  HN  LEU   375       -3.183   0.916   2.749  1.00  0.32
ATOM    797  CA  LEU   375       -2.079  -0.496   3.936  1.00  0.32
ATOM    798  HA  LEU   375       -1.630  -1.382   3.512  1.00  0.32
ATOM    799  CB  LEU   375       -1.023   0.611   4.046  1.00  0.33
ATOM    800  HB1 LEU   375       -0.468   0.483   4.962  1.00  0.39
ATOM    801  HB2 LEU   375       -1.516   1.572   4.060  1.00  0.36
ATOM    802  CG  LEU   375       -0.049   0.556   2.850  1.00  0.29
ATOM    803  HG  LEU   375        0.693  -0.208   3.028  1.00  0.34
ATOM    804  CD1 LEU   375       -0.797   0.246   1.545  1.00  0.31
ATOM    805 HD11 LEU   375       -1.039  -0.806   1.513  1.00  1.12
ATOM    806 HD12 LEU   375       -0.171   0.497   0.703  1.00  1.00
ATOM    807 HD13 LEU   375       -1.706   0.827   1.504  1.00  1.03
ATOM    808  CD2 LEU   375        0.643   1.912   2.704  1.00  0.32
ATOM    809 HD21 LEU   375        1.428   1.998   3.439  1.00  0.98
ATOM    810 HD22 LEU   375       -0.078   2.702   2.852  1.00  1.08
ATOM    811 HD23 LEU   375        1.067   1.994   1.713  1.00  1.10
ATOM    812  C   LEU   375       -2.648  -0.821   5.319  1.00  0.36
ATOM    813  O   LEU   375       -2.103  -1.619   6.055  1.00  0.40
ATOM    814  N   ALA   376       -3.746  -0.213   5.673  1.00  0.37
ATOM    815  HN  ALA   376       -4.172   0.423   5.061  1.00  0.37
ATOM    816  CA  ALA   376       -4.357  -0.490   7.002  1.00  0.43
ATOM    817  HA  ALA   376       -3.584  -0.758   7.707  1.00  0.46
ATOM    818  CB  ALA   376       -5.088   0.761   7.495  1.00  0.48
ATOM    819  HB1 ALA   376       -5.716   1.146   6.705  1.00  1.09
ATOM    820  HB2 ALA   376       -4.365   1.512   7.778  1.00  1.10
ATOM    821  HB3 ALA   376       -5.698   0.508   8.350  1.00  1.17
ATOM    822  C   ALA   376       -5.350  -1.647   6.867  1.00  0.43
ATOM    823  O   ALA   376       -5.228  -2.666   7.520  1.00  0.46
ATOM    824  N   THR   377       -6.332  -1.499   6.018  1.00  0.42
ATOM    825  HN  THR   377       -6.409  -0.672   5.498  1.00  0.43
ATOM    826  CA  THR   377       -7.331  -2.590   5.832  1.00  0.44
ATOM    827  HA  THR   377       -7.907  -2.711   6.737  1.00  0.48
ATOM    828  CB  THR   377       -8.267  -2.236   4.673  1.00  0.46
ATOM    829  HB  THR   377       -7.690  -2.116   3.769  1.00  0.60
ATOM    830  OG1 THR   377       -8.948  -1.025   4.966  1.00  0.73
ATOM    831  HG1 THR   377       -8.501  -0.313   4.502  1.00  0.87
ATOM    832  CG2 THR   377       -9.282  -3.362   4.473  1.00  0.74
ATOM    833 HG21 THR   377       -9.052  -3.896   3.563  1.00  1.30
ATOM    834 HG22 THR   377      -10.275  -2.943   4.405  1.00  1.28
ATOM    835 HG23 THR   377       -9.234  -4.042   5.311  1.00  1.34
ATOM    836  C   THR   377       -6.603  -3.895   5.510  1.00  0.41
ATOM    837  O   THR   377       -7.045  -4.968   5.864  1.00  0.46
ATOM    838  N   TRP   378       -5.489  -3.809   4.840  1.00  0.36
ATOM    839  HN  TRP   378       -5.150  -2.932   4.564  1.00  0.35
ATOM    840  CA  TRP   378       -4.730  -5.041   4.495  1.00  0.36
ATOM    841  HA  TRP   378       -5.351  -5.689   3.895  1.00  0.39
ATOM    842  CB  TRP   378       -3.478  -4.657   3.704  1.00  0.34
ATOM    843  HB1 TRP   378       -2.856  -4.015   4.309  1.00  0.36
ATOM    844  HB2 TRP   378       -3.768  -4.134   2.805  1.00  0.34
ATOM    845  CG  TRP   378       -2.717  -5.890   3.337  1.00  0.36
ATOM    846  CD1 TRP   378       -2.033  -6.669   4.207  1.00  0.46
ATOM    847  HD1 TRP   378       -1.951  -6.501   5.271  1.00  0.54
```

09854906.091401

Figure 8 (12 of 19)

```
ATOM    848  CD2 TRP   378      -2.547  -6.497   2.023  1.00  0.33
ATOM    849  NE1 TRP   378      -1.455  -7.715   3.510  1.00  0.49
ATOM    850  HE1 TRP   378      -0.906  -8.423   3.907  1.00  0.57
ATOM    851  CE2 TRP   378      -1.743  -7.652   2.162  1.00  0.40
ATOM    852  CE3 TRP   378      -3.008  -6.160   0.738  1.00  0.31
ATOM    853  HE3 TRP   378      -3.624  -5.283   0.601  1.00  0.32
ATOM    854  CZ2 TRP   378      -1.408  -8.446   1.064  1.00  0.41
ATOM    855  HZ2 TRP   378      -0.793  -9.323   1.196  1.00  0.48
ATOM    856  CZ3 TRP   378      -2.673  -6.956  -0.369  1.00  0.35
ATOM    857  HZ3 TRP   378      -3.033  -6.688  -1.352  1.00  0.39
ATOM    858  CH2 TRP   378      -1.874  -8.097  -0.206  1.00  0.38
ATOM    859  HH2 TRP   378      -1.620  -8.705  -1.061  1.00  0.42
ATOM    860  C   TRP   378      -4.325  -5.766   5.781  1.00  0.42
ATOM    861  O   TRP   378      -4.720  -6.888   6.025  1.00  0.48
ATOM    862  N   ARG   379      -3.543  -5.132   6.611  1.00  0.45
ATOM    863  HN  ARG   379      -3.237  -4.225   6.400  1.00  0.43
ATOM    864  CA  ARG   379      -3.116  -5.786   7.881  1.00  0.56
ATOM    865  HA  ARG   379      -2.458  -6.612   7.657  1.00  0.60
ATOM    866  CB  ARG   379      -2.378  -4.769   8.753  1.00  0.61
ATOM    867  HB1 ARG   379      -3.033  -4.426   9.540  1.00  1.05
ATOM    868  HB2 ARG   379      -2.074  -3.928   8.146  1.00  0.93
ATOM    869  CG  ARG   379      -1.142  -5.425   9.372  1.00  1.20
ATOM    870  HG1 ARG   379      -0.455  -5.709   8.590  1.00  1.69
ATOM    871  HG2 ARG   379      -1.441  -6.303   9.927  1.00  1.72
ATOM    872  CD  ARG   379      -0.457  -4.433  10.314  1.00  1.28
ATOM    873  HD1 ARG   379      -0.446  -3.454   9.859  1.00  1.81
ATOM    874  HD2 ARG   379       0.556  -4.755  10.501  1.00  1.54
ATOM    875  NE  ARG   379      -1.206  -4.375  11.600  1.00  1.88
ATOM    876  HE  ARG   379      -1.853  -5.076  11.823  1.00  2.50
ATOM    877  CZ  ARG   379      -1.001  -3.389  12.430  1.00  2.25
ATOM    878  NH1 ARG   379       0.175  -2.829  12.501  1.00  2.62
ATOM    879 HH11 ARG   379       0.920  -3.156  11.920  1.00  2.83
ATOM    880 HH12 ARG   379       0.332  -2.074  13.137  1.00  3.07
ATOM    881  NH2 ARG   379      -1.974  -2.962  13.188  1.00  2.89
ATOM    882 HH21 ARG   379      -2.875  -3.390  13.133  1.00  3.20
ATOM    883 HH22 ARG   379      -1.817  -2.207  13.824  1.00  3.36
ATOM    884  C   ARG   379      -4.347  -6.302   8.633  1.00  0.62
ATOM    885  O   ARG   379      -4.262  -7.219   9.426  1.00  0.72
ATOM    886  N   ARG   380      -5.489  -5.718   8.393  1.00  0.59
ATOM    887  HN  ARG   380      -5.536  -4.976   7.751  1.00  0.52
ATOM    888  CA  ARG   380      -6.721  -6.174   9.097  1.00  0.69
ATOM    889  HA  ARG   380      -6.455  -6.560  10.070  1.00  0.77
ATOM    890  CB  ARG   380      -7.678  -4.993   9.264  1.00  0.76
ATOM    891  HB1 ARG   380      -8.600  -5.198   8.740  1.00  1.26
ATOM    892  HB2 ARG   380      -7.223  -4.101   8.857  1.00  0.91
ATOM    893  CG  ARG   380      -7.976  -4.784  10.750  1.00  1.59
ATOM    894  HG1 ARG   380      -7.119  -4.336  11.229  1.00  2.10
ATOM    895  HG2 ARG   380      -8.188  -5.738  11.211  1.00  2.23
ATOM    896  CD  ARG   380      -9.185  -3.860  10.906  1.00  2.04
ATOM    897  HD1 ARG   380      -9.722  -3.809   9.971  1.00  2.37
ATOM    898  HD2 ARG   380      -8.850  -2.872  11.183  1.00  2.55
ATOM    899  NE  ARG   380     -10.084  -4.396  11.967  1.00  2.53
ATOM    900  HE  ARG   380     -10.383  -5.328  11.931  1.00  2.83
ATOM    901  CZ  ARG   380     -10.473  -3.623  12.943  1.00  3.11
ATOM    902  NH1 ARG   380     -10.311  -4.004  14.181  1.00  3.54
ATOM    903 HH11 ARG   380      -9.888  -4.887  14.381  1.00  3.57
ATOM    904 HH12 ARG   380     -10.609  -3.411  14.929  1.00  4.10
ATOM    905  NH2 ARG   380     -11.026  -2.470  12.682  1.00  3.72
ATOM    906 HH21 ARG   380     -11.152  -2.179  11.734  1.00  3.88
ATOM    907 HH22 ARG   380     -11.324  -1.878  13.431  1.00  4.28
ATOM    908  C   ARG   380      -7.410  -7.275   8.283  1.00  0.67
ATOM    909  O   ARG   380      -7.454  -8.421   8.685  1.00  0.75
ATOM    910  N   ARG   381      -7.955  -6.934   7.147  1.00  0.70
ATOM    911  HN  ARG   381      -7.914  -6.003   6.846  1.00  0.75
ATOM    912  CA  ARG   381      -8.652  -7.957   6.314  1.00  0.80
ATOM    913  HA  ARG   381      -9.469  -8.380   6.879  1.00  0.86
ATOM    914  CB  ARG   381      -9.203  -7.295   5.049  1.00  0.94
ATOM    915  HB1 ARG   381      -8.389  -7.058   4.380  1.00  1.35
ATOM    916  HB2 ARG   381      -9.725  -6.387   5.316  1.00  1.19
ATOM    917  CG  ARG   381     -10.169  -8.253   4.351  1.00  1.64
ATOM    918  HG1 ARG   381     -10.890  -8.621   5.066  1.00  2.21
ATOM    919  HG2 ARG   381      -9.616  -9.084   3.937  1.00  2.31
ATOM    920  CD  ARG   381     -10.900  -7.515   3.229  1.00  1.84
ATOM    921  HD1 ARG   381     -11.038  -8.180   2.390  1.00  2.15
ATOM    922  HD2 ARG   381     -10.314  -6.662   2.919  1.00  1.90
ATOM    923  NE  ARG   381     -12.229  -7.052   3.720  1.00  2.80
ATOM    924  HE  ARG   381     -12.322  -6.160   4.113  1.00  3.22
```

Figure 8 (13 of 19)

```
ATOM    925  CZ  ARG   381     -13.268  -7.836   3.627  1.00  3.46
ATOM    926  NH1 ARG   381     -13.493  -8.493   2.522  1.00  4.06
ATOM    927 HH11 ARG   381     -12.869  -8.396   1.747  1.00  4.12
ATOM    928 HH12 ARG   381     -14.290  -9.093   2.451  1.00  4.71
ATOM    929  NH2 ARG   381     -14.082  -7.962   4.639  1.00  3.98
ATOM    930 HH21 ARG   381     -13.910  -7.457   5.486  1.00  4.01
ATOM    931 HH22 ARG   381     -14.879  -8.562   4.569  1.00  4.63
ATOM    932  C   ARG   381      -7.676  -9.072   5.925  1.00  0.78
ATOM    933  O   ARG   381      -7.778 -10.186   6.397  1.00  0.88
ATOM    934  N   THR   382      -6.734  -8.787   5.063  1.00  0.78
ATOM    935  HN  THR   382      -6.668  -7.884   4.690  1.00  0.79
ATOM    936  CA  THR   382      -5.761  -9.841   4.646  1.00  0.86
ATOM    937  HA  THR   382      -6.276 -10.587   4.062  1.00  0.93
ATOM    938  CB  THR   382      -4.652  -9.210   3.794  1.00  1.00
ATOM    939  HB  THR   382      -3.689  -9.477   4.202  1.00  1.30
ATOM    940  OG1 THR   382      -4.792  -7.796   3.799  1.00  1.82
ATOM    941  HG1 THR   382      -5.486  -7.562   3.177  1.00  2.07
ATOM    942  CG2 THR   382      -4.751  -9.726   2.358  1.00  0.85
ATOM    943 HG21 THR   382      -3.761  -9.943   1.984  1.00  1.28
ATOM    944 HG22 THR   382      -5.214  -8.973   1.736  1.00  1.45
ATOM    945 HG23 THR   382      -5.348 -10.625   2.339  1.00  1.45
ATOM    946  C   THR   382      -5.143 -10.491   5.895  1.00  0.93
ATOM    947  O   THR   382      -4.539  -9.813   6.701  1.00  1.11
ATOM    948  N   PRO   383      -5.318 -11.788   6.025  1.00  1.10
ATOM    949  CA  PRO   383      -4.768 -12.507   7.202  1.00  1.23
ATOM    950  HA  PRO   383      -5.068 -12.024   8.117  1.00  1.37
ATOM    951  CB  PRO   383      -5.404 -13.892   7.109  1.00  1.57
ATOM    952  HB1 PRO   383      -6.305 -13.933   7.702  1.00  1.79
ATOM    953  HB2 PRO   383      -4.703 -14.649   7.433  1.00  1.68
ATOM    954  CG  PRO   383      -5.735 -14.068   5.663  1.00  1.80
ATOM    955  HG1 PRO   383      -6.607 -14.695   5.557  1.00  2.21
ATOM    956  HG2 PRO   383      -4.894 -14.508   5.145  1.00  1.98
ATOM    957  CD  PRO   383      -6.026 -12.697   5.111  1.00  1.47
ATOM    958  HD2 PRO   383      -5.638 -12.605   4.105  1.00  1.54
ATOM    959  HD1 PRO   383      -7.085 -12.494   5.132  1.00  1.64
ATOM    960  C   PRO   383      -3.243 -12.599   7.112  1.00  1.42
ATOM    961  O   PRO   383      -2.700 -13.420   6.400  1.00  1.88
ATOM    962  N   ARG   384      -2.549 -11.761   7.831  1.00  1.85
ATOM    963  HN  ARG   384      -3.008 -11.107   8.399  1.00  2.26
ATOM    964  CA  ARG   384      -1.061 -11.797   7.792  1.00  2.30
ATOM    965  HA  ARG   384      -0.732 -12.770   7.458  1.00  2.77
ATOM    966  CB  ARG   384      -0.550 -10.725   6.827  1.00  3.43
ATOM    967  HB1 ARG   384       0.519 -10.620   6.938  1.00  3.74
ATOM    968  HB2 ARG   384      -1.030  -9.783   7.049  1.00  3.69
ATOM    969  CG  ARG   384      -0.871 -11.137   5.388  1.00  4.37
ATOM    970  HG1 ARG   384      -0.986 -10.253   4.778  1.00  4.65
ATOM    971  HG2 ARG   384      -1.789 -11.707   5.373  1.00  4.55
ATOM    972  CD  ARG   384       0.271 -11.990   4.833  1.00  5.29
ATOM    973  HD1 ARG   384       1.111 -11.949   5.509  1.00  5.62
ATOM    974  HD2 ARG   384       0.567 -11.610   3.867  1.00  5.43
ATOM    975  NE  ARG   384      -0.185 -13.402   4.692  1.00  6.06
ATOM    976  HE  ARG   384      -0.989 -13.609   4.170  1.00  6.11
ATOM    977  CZ  ARG   384       0.487 -14.364   5.264  1.00  6.93
ATOM    978  NH1 ARG   384       1.790 -14.311   5.312  1.00  7.58
ATOM    979 HH11 ARG   384       2.274 -13.533   4.910  1.00  7.49
ATOM    980 HH12 ARG   384       2.305 -15.048   5.751  1.00  8.31
ATOM    981  NH2 ARG   384      -0.144 -15.379   5.788  1.00  7.38
ATOM    982 HH21 ARG   384      -1.143 -15.420   5.752  1.00  7.11
ATOM    983 HH22 ARG   384       0.371 -16.116   6.227  1.00  8.15
ATOM    984  C   ARG   384      -0.514 -11.526   9.195  1.00  1.73
ATOM    985  O   ARG   384      -1.260 -11.365  10.140  1.00  2.21
ATOM    986  N   ARG   385       0.781 -11.476   9.342  1.00  1.68
ATOM    987  HN  ARG   385       1.369 -11.610   8.569  1.00  2.10
ATOM    988  CA  ARG   385       1.365 -11.218  10.688  1.00  2.09
ATOM    989  HA  ARG   385       0.571 -11.017  11.391  1.00  2.63
ATOM    990  CB  ARG   385       2.152 -12.447  11.146  1.00  3.06
ATOM    991  HB1 ARG   385       2.872 -12.155  11.896  1.00  3.55
ATOM    992  HB2 ARG   385       2.666 -12.881  10.301  1.00  3.42
ATOM    993  CG  ARG   385       1.189 -13.476  11.741  1.00  3.71
ATOM    994  HG1 ARG   385       0.884 -14.170  10.972  1.00  3.74
ATOM    995  HG2 ARG   385       0.320 -12.969  12.136  1.00  3.90
ATOM    996  CD  ARG   385       1.889 -14.242  12.866  1.00  4.81
ATOM    997  HD1 ARG   385       1.547 -13.871  13.821  1.00  5.22
ATOM    998  HD2 ARG   385       2.956 -14.101  12.787  1.00  5.16
ATOM    999  NE  ARG   385       1.568 -15.693  12.752  1.00  5.34
ATOM   1000  HE  ARG   385       0.752 -16.047  13.163  1.00  5.22
ATOM   1001  CZ  ARG   385       2.374 -16.491  12.107  1.00  6.28
```

Figure 8 (14 of 19)

```
ATOM   1002  NH1 ARG   385        2.062 -16.904  10.909  1.00  6.85
ATOM   1003 HH11 ARG   385        1.205 -16.609  10.485  1.00  6.65
ATOM   1004 HH12 ARG   385        2.679 -17.516  10.414  1.00  7.64
ATOM   1005  NH2 ARG   385        3.491 -16.877  12.661  1.00  6.90
ATOM   1006 HH21 ARG   385        3.728 -16.561  13.579  1.00  6.75
ATOM   1007 HH22 ARG   385        4.110 -17.487  12.167  1.00  7.68
ATOM   1008  C   ARG   385        2.301 -10.010  10.619  1.00  1.75
ATOM   1009  O   ARG   385        1.934  -8.907  10.970  1.00  2.29
ATOM   1010  N   GLU   386        3.509 -10.211  10.170  1.00  1.72
ATOM   1011  HN  GLU   386        3.785 -11.109   9.893  1.00  2.03
ATOM   1012  CA  GLU   386        4.469  -9.075  10.081  1.00  2.15
ATOM   1013  HA  GLU   386        3.947  -8.147  10.260  1.00  2.64
ATOM   1014  CB  GLU   386        5.568  -9.254  11.130  1.00  3.20
ATOM   1015  HB1 GLU   386        6.296  -8.464  11.027  1.00  3.64
ATOM   1016  HB2 GLU   386        6.049 -10.210  10.987  1.00  3.43
ATOM   1017  CG  GLU   386        4.952  -9.196  12.530  1.00  4.00
ATOM   1018  HG1 GLU   386        3.878  -9.130  12.447  1.00  4.00
ATOM   1019  HG2 GLU   386        5.328  -8.329  13.052  1.00  4.22
ATOM   1020  CD  GLU   386        5.324 -10.461  13.306  1.00  5.05
ATOM   1021  OE1 GLU   386        5.062 -11.541  12.802  1.00  5.61
ATOM   1022  OE2 GLU   386        5.863 -10.328  14.393  1.00  5.55
ATOM   1023  C   GLU   386        5.094  -9.049   8.685  1.00  1.56
ATOM   1024  O   GLU   386        6.196  -8.571   8.497  1.00  2.12
ATOM   1025  N   ALA   387        4.400  -9.560   7.706  1.00  1.11
ATOM   1026  HN  ALA   387        3.514  -9.941   7.880  1.00  1.61
ATOM   1027  CA  ALA   387        4.956  -9.567   6.324  1.00  0.92
ATOM   1028  HA  ALA   387        5.998  -9.284   6.355  1.00  1.12
ATOM   1029  CB  ALA   387        4.827 -10.971   5.731  1.00  1.44
ATOM   1030  HB1 ALA   387        3.867 -11.069   5.245  1.00  1.84
ATOM   1031  HB2 ALA   387        4.908 -11.704   6.519  1.00  2.02
ATOM   1032  HB3 ALA   387        5.614 -11.130   5.009  1.00  1.84
ATOM   1033  C   ALA   387        4.183  -8.572   5.455  1.00  0.77
ATOM   1034  O   ALA   387        4.175  -8.669   4.244  1.00  0.70
ATOM   1035  N   THR   388        3.534  -7.613   6.060  1.00  0.76
ATOM   1036  HN  THR   388        3.552  -7.549   7.038  1.00  0.83
ATOM   1037  CA  THR   388        2.767  -6.616   5.262  1.00  0.68
ATOM   1038  HA  THR   388        1.959  -7.112   4.744  1.00  0.72
ATOM   1039  CB  THR   388        2.195  -5.546   6.196  1.00  0.78
ATOM   1040  HB  THR   388        2.773  -4.639   6.104  1.00  1.34
ATOM   1041  OG1 THR   388        2.253  -6.012   7.537  1.00  1.54
ATOM   1042  HG1 THR   388        1.699  -5.440   8.074  1.00  1.90
ATOM   1043  CG2 THR   388        0.742  -5.257   5.815  1.00  1.16
ATOM   1044 HG21 THR   388        0.491  -4.244   6.093  1.00  1.67
ATOM   1045 HG22 THR   388        0.090  -5.945   6.335  1.00  1.72
ATOM   1046 HG23 THR   388        0.618  -5.380   4.750  1.00  1.78
ATOM   1047  C   THR   388        3.700  -5.960   4.242  1.00  0.54
ATOM   1048  O   THR   388        3.564  -6.148   3.049  1.00  0.50
ATOM   1049  N   LEU   389        4.653  -5.195   4.702  1.00  0.52
ATOM   1050  HN  LEU   389        4.749  -5.059   5.668  1.00  0.59
ATOM   1051  CA  LEU   389        5.600  -4.531   3.760  1.00  0.46
ATOM   1052  HA  LEU   389        5.064  -3.810   3.156  1.00  0.44
ATOM   1053  CB  LEU   389        6.692  -3.818   4.558  1.00  0.52
ATOM   1054  HB1 LEU   389        7.238  -4.541   5.145  1.00  0.87
ATOM   1055  HB2 LEU   389        6.240  -3.090   5.214  1.00  0.98
ATOM   1056  CG  LEU   389        7.654  -3.116   3.597  1.00  0.62
ATOM   1057  HG  LEU   389        7.889  -3.779   2.776  1.00  1.22
ATOM   1058  CD1 LEU   389        7.001  -1.844   3.053  1.00  1.13
ATOM   1059 HD11 LEU   389        7.690  -1.018   3.146  1.00  1.65
ATOM   1060 HD12 LEU   389        6.105  -1.630   3.616  1.00  1.62
ATOM   1061 HD13 LEU   389        6.747  -1.986   2.013  1.00  1.72
ATOM   1062  CD2 LEU   389        8.938  -2.749   4.343  1.00  1.15
ATOM   1063 HD21 LEU   389        8.712  -2.577   5.385  1.00  1.68
ATOM   1064 HD22 LEU   389        9.360  -1.853   3.913  1.00  1.74
ATOM   1065 HD23 LEU   389        9.648  -3.558   4.257  1.00  1.62
ATOM   1066  C   LEU   389        6.240  -5.587   2.855  1.00  0.45
ATOM   1067  O   LEU   389        6.573  -5.323   1.718  1.00  0.43
ATOM   1068  N   GLU   390        6.412  -6.783   3.353  1.00  0.50
ATOM   1069  HN  GLU   390        6.134  -6.975   4.273  1.00  0.54
ATOM   1070  CA  GLU   390        7.027  -7.858   2.522  1.00  0.53
ATOM   1071  HA  GLU   390        8.054  -7.602   2.303  1.00  0.56
ATOM   1072  CB  GLU   390        6.983  -9.183   3.288  1.00  0.63
ATOM   1073  HB1 GLU   390        6.023  -9.653   3.139  1.00  0.99
ATOM   1074  HB2 GLU   390        7.133  -8.995   4.341  1.00  1.10
ATOM   1075  CG  GLU   390        8.086 -10.111   2.772  1.00  1.11
ATOM   1076  HG1 GLU   390        8.922  -9.521   2.430  1.00  1.76
ATOM   1077  HG2 GLU   390        7.704 -10.705   1.955  1.00  1.71
ATOM   1078  CD  GLU   390        8.547 -11.034   3.902  1.00  1.45
```

Figure 8 (15 of 19)

```
ATOM   1079  OE1 GLU   390       8.935 -12.152   3.606  1.00  1.95
ATOM   1080  OE2 GLU   390       8.505 -10.607   5.044  1.00  2.14
ATOM   1081  C   GLU   390       6.245  -7.994   1.215  1.00  0.46
ATOM   1082  O   GLU   390       6.763  -7.757   0.142  1.00  0.46
ATOM   1083  N   LEU   391       4.995  -8.361   1.297  1.00  0.44
ATOM   1084  HN  LEU   391       4.591  -8.539   2.172  1.00  0.48
ATOM   1085  CA  LEU   391       4.181  -8.495   0.058  1.00  0.41
ATOM   1086  HA  LEU   391       4.603  -9.265  -0.572  1.00  0.43
ATOM   1087  CB  LEU   391       2.743  -8.865   0.428  1.00  0.45
ATOM   1088  HB1 LEU   391       2.265  -8.022   0.903  1.00  0.49
ATOM   1089  HB2 LEU   391       2.751  -9.705   1.108  1.00  0.47
ATOM   1090  CG  LEU   391       1.972  -9.239  -0.838  1.00  0.47
ATOM   1091  HG  LEU   391       2.668  -9.552  -1.602  1.00  0.76
ATOM   1092  CD1 LEU   391       1.005 -10.383  -0.531  1.00  1.11
ATOM   1093 HD11 LEU   391       0.001  -9.994  -0.452  1.00  1.62
ATOM   1094 HD12 LEU   391       1.284 -10.851   0.402  1.00  1.81
ATOM   1095 HD13 LEU   391       1.047 -11.113  -1.326  1.00  1.44
ATOM   1096  CD2 LEU   391       1.185  -8.023  -1.328  1.00  0.85
ATOM   1097 HD21 LEU   391       0.518  -7.688  -0.547  1.00  1.46
ATOM   1098 HD22 LEU   391       0.610  -8.295  -2.199  1.00  1.50
ATOM   1099 HD23 LEU   391       1.870  -7.228  -1.582  1.00  1.36
ATOM   1100  C   LEU   391       4.194  -7.159  -0.686  1.00  0.35
ATOM   1101  O   LEU   391       4.257  -7.110  -1.898  1.00  0.34
ATOM   1102  N   LEU   392       4.149  -6.073   0.038  1.00  0.33
ATOM   1103  HN  LEU   392       4.109  -6.138   1.015  1.00  0.36
ATOM   1104  CA  LEU   392       4.175  -4.736  -0.617  1.00  0.30
ATOM   1105  HA  LEU   392       3.376  -4.667  -1.341  1.00  0.30
ATOM   1106  CB  LEU   392       4.007  -3.646   0.445  1.00  0.31
ATOM   1107  HB1 LEU   392       4.383  -2.709   0.066  1.00  0.30
ATOM   1108  HB2 LEU   392       4.562  -3.923   1.326  1.00  0.35
ATOM   1109  CG  LEU   392       2.527  -3.490   0.807  1.00  0.33
ATOM   1110  HG  LEU   392       1.967  -4.321   0.404  1.00  0.41
ATOM   1111  CD1 LEU   392       2.380  -3.464   2.329  1.00  0.45
ATOM   1112 HD11 LEU   392       3.283  -3.068   2.770  1.00  1.16
ATOM   1113 HD12 LEU   392       2.211  -4.467   2.691  1.00  1.11
ATOM   1114 HD13 LEU   392       1.543  -2.837   2.599  1.00  1.10
ATOM   1115  CD2 LEU   392       1.990  -2.177   0.227  1.00  0.28
ATOM   1116 HD21 LEU   392       0.990  -2.003   0.596  1.00  1.06
ATOM   1117 HD22 LEU   392       1.970  -2.239  -0.851  1.00  1.01
ATOM   1118 HD23 LEU   392       2.631  -1.361   0.528  1.00  1.01
ATOM   1119  C   LEU   392       5.524  -4.555  -1.317  1.00  0.29
ATOM   1120  O   LEU   392       5.638  -3.856  -2.304  1.00  0.30
ATOM   1121  N   GLY   393       6.550  -5.182  -0.805  1.00  0.31
ATOM   1122  HN  GLY   393       6.433  -5.738  -0.007  1.00  0.32
ATOM   1123  CA  GLY   393       7.898  -5.053  -1.428  1.00  0.33
ATOM   1124  HA1 GLY   393       8.629  -5.549  -0.808  1.00  0.37
ATOM   1125  HA2 GLY   393       8.154  -4.007  -1.519  1.00  0.33
ATOM   1126  C   GLY   393       7.891  -5.700  -2.813  1.00  0.34
ATOM   1127  O   GLY   393       8.163  -5.059  -3.808  1.00  0.34
ATOM   1128  N   ARG   394       7.579  -6.965  -2.892  1.00  0.36
ATOM   1129  HN  ARG   394       7.359  -7.469  -2.080  1.00  0.37
ATOM   1130  CA  ARG   394       7.553  -7.641  -4.222  1.00  0.39
ATOM   1131  HA  ARG   394       8.555  -7.683  -4.625  1.00  0.42
ATOM   1132  CB  ARG   394       7.003  -9.060  -4.066  1.00  0.42
ATOM   1133  HB1 ARG   394       6.227  -9.228  -4.798  1.00  0.92
ATOM   1134  HB2 ARG   394       6.594  -9.179  -3.073  1.00  1.01
ATOM   1135  CG  ARG   394       8.130 -10.072  -4.280  1.00  1.21
ATOM   1136  HG1 ARG   394       8.683 -10.194  -3.361  1.00  1.76
ATOM   1137  HG2 ARG   394       8.793  -9.714  -5.054  1.00  1.89
ATOM   1138  CD  ARG   394       7.535 -11.418  -4.697  1.00  1.42
ATOM   1139  HD1 ARG   394       8.232 -11.935  -5.341  1.00  1.92
ATOM   1140  HD2 ARG   394       6.609 -11.254  -5.227  1.00  1.64
ATOM   1141  NE  ARG   394       7.274 -12.243  -3.484  1.00  2.11
ATOM   1142  HE  ARG   394       7.059 -11.808  -2.632  1.00  2.52
ATOM   1143  CZ  ARG   394       7.331 -13.544  -3.555  1.00  2.76
ATOM   1144  NH1 ARG   394       7.764 -14.235  -2.536  1.00  3.24
ATOM   1145 HH11 ARG   394       8.051 -13.768  -1.700  1.00  3.28
ATOM   1146 HH12 ARG   394       7.808 -15.233  -2.591  1.00  3.88
ATOM   1147  NH2 ARG   394       6.956 -14.155  -4.646  1.00  3.46
ATOM   1148 HH21 ARG   394       6.624 -13.625  -5.426  1.00  3.60
ATOM   1149 HH22 ARG   394       7.000 -15.152  -4.701  1.00  4.12
ATOM   1150  C   ARG   394       6.654  -6.846  -5.170  1.00  0.36
ATOM   1151  O   ARG   394       6.957  -6.667  -6.334  1.00  0.38
ATOM   1152  N   VAL   395       5.553  -6.358  -4.671  1.00  0.33
ATOM   1153  HN  VAL   395       5.335  -6.508  -3.728  1.00  0.32
ATOM   1154  CA  VAL   395       4.634  -5.564  -5.528  1.00  0.33
ATOM   1155  HA  VAL   395       4.353  -6.145  -6.394  1.00  0.37
```

```
ATOM   1156  CB  VAL   395        3.384  -5.204  -4.725  1.00  0.32
ATOM   1157  HB  VAL   395        3.666  -4.607  -3.870  1.00  0.29
ATOM   1158  CG1 VAL   395        2.417  -4.411  -5.606  1.00  0.36
ATOM   1159 HG11 VAL   395        2.979  -3.803  -6.300  1.00  0.97
ATOM   1160 HG12 VAL   395        1.803  -3.775  -4.985  1.00  1.08
ATOM   1161 HG13 VAL   395        1.787  -5.095  -6.155  1.00  1.17
ATOM   1162  CG2 VAL   395        2.704  -6.489  -4.247  1.00  0.35
ATOM   1163 HG21 VAL   395        2.051  -6.861  -5.023  1.00  1.13
ATOM   1164 HG22 VAL   395        2.126  -6.281  -3.359  1.00  1.00
ATOM   1165 HG23 VAL   395        3.455  -7.231  -4.022  1.00  1.08
ATOM   1166  C   VAL   395        5.349  -4.289  -5.976  1.00  0.31
ATOM   1167  O   VAL   395        5.053  -3.728  -7.012  1.00  0.34
ATOM   1168  N   LEU   396        6.299  -3.833  -5.204  1.00  0.28
ATOM   1169  HN  LEU   396        6.526  -4.307  -4.376  1.00  0.27
ATOM   1170  CA  LEU   396        7.046  -2.602  -5.584  1.00  0.28
ATOM   1171  HA  LEU   396        6.355  -1.851  -5.937  1.00  0.29
ATOM   1172  CB  LEU   396        7.812  -2.069  -4.371  1.00  0.26
ATOM   1173  HB1 LEU   396        8.578  -1.385  -4.702  1.00  0.27
ATOM   1174  HB2 LEU   396        8.271  -2.892  -3.845  1.00  0.28
ATOM   1175  CG  LEU   396        6.852  -1.339  -3.431  1.00  0.25
ATOM   1176  HG  LEU   396        5.961  -1.934  -3.293  1.00  0.27
ATOM   1177  CD1 LEU   396        7.533  -1.116  -2.081  1.00  0.27
ATOM   1178 HD11 LEU   396        7.377  -0.096  -1.763  1.00  0.89
ATOM   1179 HD12 LEU   396        8.592  -1.305  -2.177  1.00  1.01
ATOM   1180 HD13 LEU   396        7.112  -1.790  -1.350  1.00  0.97
ATOM   1181  CD2 LEU   396        6.477   0.014  -4.036  1.00  0.27
ATOM   1182 HD21 LEU   396        7.257   0.731  -3.826  1.00  0.97
ATOM   1183 HD22 LEU   396        5.549   0.355  -3.603  1.00  1.11
ATOM   1184 HD23 LEU   396        6.361  -0.089  -5.103  1.00  0.99
ATOM   1185  C   LEU   396        8.042  -2.946  -6.692  1.00  0.32
ATOM   1186  O   LEU   396        8.150  -2.253  -7.684  1.00  0.34
ATOM   1187  N   ARG   397        8.772  -4.017  -6.526  1.00  0.34
ATOM   1188  HN  ARG   397        8.666  -4.557  -5.715  1.00  0.34
ATOM   1189  CA  ARG   397        9.768  -4.420  -7.561  1.00  0.40
ATOM   1190  HA  ARG   397       10.582  -3.710  -7.573  1.00  0.41
ATOM   1191  CB  ARG   397       10.311  -5.811  -7.228  1.00  0.46
ATOM   1192  HB1 ARG   397       10.691  -6.274  -8.127  1.00  0.88
ATOM   1193  HB2 ARG   397        9.517  -6.418  -6.818  1.00  0.90
ATOM   1194  CG  ARG   397       11.440  -5.687  -6.204  1.00  1.21
ATOM   1195  HG1 ARG   397       11.190  -4.923  -5.483  1.00  1.73
ATOM   1196  HG2 ARG   397       12.357  -5.419  -6.709  1.00  1.81
ATOM   1197  CD  ARG   397       11.626  -7.024  -5.483  1.00  1.32
ATOM   1198  HD1 ARG   397       10.791  -7.672  -5.705  1.00  1.65
ATOM   1199  HD2 ARG   397       11.676  -6.854  -4.418  1.00  1.83
ATOM   1200  NE  ARG   397       12.889  -7.666  -5.943  1.00  1.97
ATOM   1201  HE  ARG   397       13.550  -7.144  -6.443  1.00  2.54
ATOM   1202  CZ  ARG   397       13.114  -8.924  -5.679  1.00  2.26
ATOM   1203  NH1 ARG   397       12.165  -9.805  -5.842  1.00  2.65
ATOM   1204 HH11 ARG   397       11.265  -9.516  -6.168  1.00  3.00
ATOM   1205 HH12 ARG   397       12.338 -10.769  -5.640  1.00  2.88
ATOM   1206  NH2 ARG   397       14.289  -9.301  -5.253  1.00  2.68
ATOM   1207 HH21 ARG   397       15.016  -8.626  -5.129  1.00  3.03
ATOM   1208 HH22 ARG   397       14.461 -10.265  -5.051  1.00  2.94
ATOM   1209  C   ARG   397        9.100  -4.450  -8.938  1.00  0.43
ATOM   1210  O   ARG   397        9.626  -3.935  -9.904  1.00  0.46
ATOM   1211  N   ASP   398        7.941  -5.046  -9.035  1.00  0.45
ATOM   1212  HN  ASP   398        7.530  -5.454  -8.242  1.00  0.44
ATOM   1213  CA  ASP   398        7.242  -5.101 -10.351  1.00  0.51
ATOM   1214  HA  ASP   398        7.815  -5.706 -11.039  1.00  0.57
ATOM   1215  CB  ASP   398        5.853  -5.715 -10.165  1.00  0.56
ATOM   1216  HB1 ASP   398        5.241  -5.488 -11.026  1.00  1.02
ATOM   1217  HB2 ASP   398        5.394  -5.303  -9.278  1.00  0.99
ATOM   1218  CG  ASP   398        5.978  -7.233 -10.018  1.00  1.21
ATOM   1219  OD1 ASP   398        5.076  -7.829  -9.454  1.00  1.79
ATOM   1220  OD2 ASP   398        6.974  -7.772 -10.472  1.00  2.00
ATOM   1221  C   ASP   398        7.103  -3.683 -10.912  1.00  0.49
ATOM   1222  O   ASP   398        7.243  -3.455 -12.097  1.00  0.54
ATOM   1223  N   MET   399        6.833  -2.728 -10.064  1.00  0.45
ATOM   1224  HN  MET   399        6.728  -2.936  -9.112  1.00  0.43
ATOM   1225  CA  MET   399        6.687  -1.322 -10.538  1.00  0.48
ATOM   1226  HA  MET   399        6.314  -1.319 -11.550  1.00  0.55
ATOM   1227  CB  MET   399        5.700  -0.586  -9.636  1.00  0.51
ATOM   1228  HB1 MET   399        5.519   0.401 -10.031  1.00  0.86
ATOM   1229  HB2 MET   399        6.113  -0.507  -8.640  1.00  1.11
ATOM   1230  CG  MET   399        4.385  -1.363  -9.585  1.00  1.30
ATOM   1231  HG1 MET   399        4.593  -2.415  -9.458  1.00  2.02
ATOM   1232  HG2 MET   399        3.841  -1.212 -10.505  1.00  1.97
```

Figure 8 (17 of 19)

```
ATOM   1233  SD  MET   399      3.394  -0.773  -8.193  1.00  1.54
ATOM   1234  CE  MET   399      3.224   0.938  -8.751  1.00  0.65
ATOM   1235  HE1 MET   399      3.734   1.060  -9.696  1.00  1.39
ATOM   1236  HE2 MET   399      3.660   1.600  -8.021  1.00  1.20
ATOM   1237  HE3 MET   399      2.176   1.174  -8.868  1.00  1.17
ATOM   1238  C   MET   399      8.045  -0.613 -10.489  1.00  0.43
ATOM   1239  O   MET   399      8.121   0.598 -10.545  1.00  0.46
ATOM   1240  N   ASP   400      9.118  -1.351 -10.384  1.00  0.40
ATOM   1241  HN  ASP   400      9.042  -2.326 -10.339  1.00  0.41
ATOM   1242  CA  ASP   400     10.459  -0.705 -10.330  1.00  0.40
ATOM   1243  HA  ASP   400     11.219  -1.463 -10.206  1.00  0.41
ATOM   1244  CB  ASP   400     10.710   0.061 -11.630  1.00  0.47
ATOM   1245  HB1 ASP   400     11.672   0.548 -11.581  1.00  0.73
ATOM   1246  HB2 ASP   400      9.937   0.804 -11.764  1.00  0.88
ATOM   1247  CG  ASP   400     10.693  -0.912 -12.810  1.00  0.97
ATOM   1248  OD1 ASP   400     11.672  -0.948 -13.537  1.00  1.34
ATOM   1249  OD2 ASP   400      9.701  -1.604 -12.966  1.00  1.85
ATOM   1250  C   ASP   400     10.510   0.267  -9.149  1.00  0.36
ATOM   1251  O   ASP   400     11.188   1.274  -9.193  1.00  0.37
ATOM   1252  N   LEU   401      9.800  -0.024  -8.094  1.00  0.34
ATOM   1253  HN  LEU   401      9.258  -0.841  -8.075  1.00  0.35
ATOM   1254  CA  LEU   401      9.813   0.890  -6.917  1.00  0.33
ATOM   1255  HA  LEU   401     10.077   1.886  -7.240  1.00  0.36
ATOM   1256  CB  LEU   401      8.428   0.917  -6.271  1.00  0.33
ATOM   1257  HB1 LEU   401      8.523   1.189  -5.230  1.00  0.36
ATOM   1258  HB2 LEU   401      7.975  -0.059  -6.348  1.00  0.36
ATOM   1259  CG  LEU   401      7.556   1.946  -6.985  1.00  0.47
ATOM   1260  HG  LEU   401      7.856   2.015  -8.021  1.00  0.91
ATOM   1261  CD1 LEU   401      6.091   1.517  -6.906  1.00  0.70
ATOM   1262 HD11 LEU   401      5.548   1.935  -7.740  1.00  1.17
ATOM   1263 HD12 LEU   401      5.661   1.873  -5.981  1.00  1.23
ATOM   1264 HD13 LEU   401      6.029   0.439  -6.940  1.00  1.25
ATOM   1265  CD2 LEU   401      7.726   3.307  -6.309  1.00  0.82
ATOM   1266 HD21 LEU   401      7.166   4.053  -6.854  1.00  1.42
ATOM   1267 HD22 LEU   401      8.772   3.576  -6.301  1.00  1.46
ATOM   1268 HD23 LEU   401      7.361   3.253  -5.294  1.00  1.31
ATOM   1269  C   LEU   401     10.837   0.400  -5.894  1.00  0.33
ATOM   1270  O   LEU   401     10.785   0.757  -4.733  1.00  0.31
ATOM   1271  N   LEU   402     11.773  -0.411  -6.308  1.00  0.39
ATOM   1272  HN  LEU   402     11.804  -0.688  -7.248  1.00  0.42
ATOM   1273  CA  LEU   402     12.796  -0.912  -5.349  1.00  0.45
ATOM   1274  HA  LEU   402     12.320  -1.532  -4.602  1.00  0.44
ATOM   1275  CB  LEU   402     13.846  -1.730  -6.101  1.00  0.55
ATOM   1276  HB1 LEU   402     14.518  -1.064  -6.621  1.00  0.93
ATOM   1277  HB2 LEU   402     13.354  -2.377  -6.814  1.00  1.19
ATOM   1278  CG  LEU   402     14.639  -2.576  -5.106  1.00  1.14
ATOM   1279  HG  LEU   402     14.834  -1.995  -4.216  1.00  1.96
ATOM   1280  CD1 LEU   402     13.828  -3.819  -4.736  1.00  1.69
ATOM   1281 HD11 LEU   402     14.473  -4.685  -4.746  1.00  2.17
ATOM   1282 HD12 LEU   402     13.031  -3.955  -5.452  1.00  2.06
ATOM   1283 HD13 LEU   402     13.408  -3.694  -3.749  1.00  2.23
ATOM   1284  CD2 LEU   402     15.963  -3.001  -5.743  1.00  1.59
ATOM   1285 HD21 LEU   402     15.922  -2.826  -6.808  1.00  2.21
ATOM   1286 HD22 LEU   402     16.131  -4.052  -5.557  1.00  1.82
ATOM   1287 HD23 LEU   402     16.770  -2.426  -5.315  1.00  2.16
ATOM   1288  C   LEU   402     13.468   0.280  -4.666  1.00  0.45
ATOM   1289  O   LEU   402     13.894   0.201  -3.531  1.00  0.47
ATOM   1290  N   GLY   403     13.567   1.392  -5.346  1.00  0.46
ATOM   1291  HN  GLY   403     13.187   1.439  -6.256  1.00  0.46
ATOM   1292  CA  GLY   403     14.176   2.594  -4.729  1.00  0.50
ATOM   1293  HA1 GLY   403     14.315   3.357  -5.479  1.00  0.55
ATOM   1294  HA2 GLY   403     15.131   2.325  -4.299  1.00  0.56
ATOM   1295  C   GLY   403     13.245   3.117  -3.638  1.00  0.43
ATOM   1296  O   GLY   403     13.673   3.703  -2.664  1.00  0.46
ATOM   1297  N   CYS   404     11.969   2.896  -3.797  1.00  0.37
ATOM   1298  HN  CYS   404     11.651   2.415  -4.589  1.00  0.37
ATOM   1299  CA  CYS   404     10.995   3.363  -2.775  1.00  0.33
ATOM   1300  HA  CYS   404     11.229   4.377  -2.488  1.00  0.38
ATOM   1301  CB  CYS   404      9.584   3.310  -3.361  1.00  0.33
ATOM   1302  HB1 CYS   404      8.876   3.083  -2.578  1.00  0.64
ATOM   1303  HB2 CYS   404      9.538   2.543  -4.121  1.00  0.55
ATOM   1304  SG  CYS   404      9.180   4.914  -4.097  1.00  0.80
ATOM   1305  HG  CYS   404      8.241   5.070  -3.972  1.00  1.29
ATOM   1306  C   CYS   404     11.081   2.456  -1.550  1.00  0.28
ATOM   1307  O   CYS   404     10.943   2.900  -0.427  1.00  0.27
ATOM   1308  N   LEU   405     11.320   1.188  -1.750  1.00  0.27
ATOM   1309  HN  LEU   405     11.437   0.847  -2.661  1.00  0.29
```

```
ATOM   1310  CA  LEU   405      11.425   0.269  -0.586  1.00  0.25
ATOM   1311  HA  LEU   405      10.552   0.380   0.038  1.00  0.25
ATOM   1312  CB  LEU   405      11.533  -1.180  -1.067  1.00  0.28
ATOM   1313  HB1 LEU   405      12.569  -1.425  -1.241  1.00  0.32
ATOM   1314  HB2 LEU   405      10.975  -1.297  -1.985  1.00  0.28
ATOM   1315  CG  LEU   405      10.961  -2.118   0.001  1.00  0.33
ATOM   1316  HG  LEU   405      11.078  -3.143  -0.321  1.00  0.97
ATOM   1317  CD1 LEU   405      11.708  -1.912   1.321  1.00  1.12
ATOM   1318 HD11 LEU   405      12.739  -1.664   1.117  1.00  1.80
ATOM   1319 HD12 LEU   405      11.663  -2.818   1.906  1.00  1.60
ATOM   1320 HD13 LEU   405      11.247  -1.105   1.873  1.00  1.61
ATOM   1321  CD2 LEU   405       9.475  -1.813   0.208  1.00  1.02
ATOM   1322 HD21 LEU   405       8.884  -2.645  -0.144  1.00  1.72
ATOM   1323 HD22 LEU   405       9.209  -0.925  -0.343  1.00  1.62
ATOM   1324 HD23 LEU   405       9.283  -1.655   1.259  1.00  1.44
ATOM   1325  C   LEU   405      12.668   0.638   0.218  1.00  0.27
ATOM   1326  O   LEU   405      12.673   0.578   1.429  1.00  0.27
ATOM   1327  N   GLU   406      13.719   1.037  -0.442  1.00  0.32
ATOM   1328  HN  GLU   406      13.695   1.093  -1.421  1.00  0.33
ATOM   1329  CA  GLU   406      14.946   1.430   0.299  1.00  0.35
ATOM   1330  HA  GLU   406      15.267   0.615   0.933  1.00  0.36
ATOM   1331  CB  GLU   406      16.055   1.785  -0.694  1.00  0.42
ATOM   1332  HB1 GLU   406      16.546   2.692  -0.376  1.00  1.01
ATOM   1333  HB2 GLU   406      15.625   1.933  -1.675  1.00  0.87
ATOM   1334  CG  GLU   406      17.076   0.647  -0.751  1.00  1.18
ATOM   1335  HG1 GLU   406      16.571  -0.277  -0.988  1.00  1.67
ATOM   1336  HG2 GLU   406      17.565   0.556   0.208  1.00  1.75
ATOM   1337  CD  GLU   406      18.117   0.949  -1.830  1.00  1.21
ATOM   1338  OE1 GLU   406      18.351   2.117  -2.089  1.00  1.59
ATOM   1339  OE2 GLU   406      18.662   0.005  -2.379  1.00  1.61
ATOM   1340  C   GLU   406      14.613   2.647   1.158  1.00  0.34
ATOM   1341  O   GLU   406      14.937   2.705   2.328  1.00  0.35
ATOM   1342  N   ASP   407      13.945   3.613   0.588  1.00  0.33
ATOM   1343  HN  ASP   407      13.680   3.537  -0.353  1.00  0.34
ATOM   1344  CA  ASP   407      13.565   4.817   1.373  1.00  0.34
ATOM   1345  HA  ASP   407      14.448   5.256   1.815  1.00  0.37
ATOM   1346  CB  ASP   407      12.888   5.833   0.447  1.00  0.36
ATOM   1347  HB1 ASP   407      12.063   5.360  -0.066  1.00  0.34
ATOM   1348  HB2 ASP   407      13.606   6.188  -0.279  1.00  0.40
ATOM   1349  CG  ASP   407      12.367   7.016   1.267  1.00  0.40
ATOM   1350  OD1 ASP   407      11.348   6.856   1.919  1.00  1.23
ATOM   1351  OD2 ASP   407      12.997   8.060   1.230  1.00  1.07
ATOM   1352  C   ASP   407      12.598   4.385   2.477  1.00  0.30
ATOM   1353  O   ASP   407      12.734   4.764   3.623  1.00  0.31
ATOM   1354  N   ILE   408      11.632   3.574   2.138  1.00  0.29
ATOM   1355  HN  ILE   408      11.551   3.270   1.211  1.00  0.30
ATOM   1356  CA  ILE   408      10.665   3.093   3.164  1.00  0.28
ATOM   1357  HA  ILE   408      10.191   3.935   3.644  1.00  0.30
ATOM   1358  CB  ILE   408       9.609   2.213   2.491  1.00  0.29
ATOM   1359  HB  ILE   408      10.093   1.374   2.013  1.00  0.30
ATOM   1360  CG1 ILE   408       8.855   3.034   1.442  1.00  0.27
ATOM   1361 HG11 ILE   408       9.502   3.807   1.057  1.00  0.29
ATOM   1362 HG12 ILE   408       7.983   3.484   1.894  1.00  0.30
ATOM   1363  CG2 ILE   408       8.623   1.698   3.541  1.00  0.35
ATOM   1364 HG21 ILE   408       8.873   2.116   4.505  1.00  1.07
ATOM   1365 HG22 ILE   408       8.680   0.621   3.590  1.00  1.11
ATOM   1366 HG23 ILE   408       7.621   1.994   3.269  1.00  1.05
ATOM   1367  CD1 ILE   408       8.420   2.121   0.295  1.00  0.25
ATOM   1368 HD11 ILE   408       7.341   2.079   0.257  1.00  0.98
ATOM   1369 HD12 ILE   408       8.813   1.128   0.457  1.00  1.11
ATOM   1370 HD13 ILE   408       8.798   2.510  -0.639  1.00  0.97
ATOM   1371  C   ILE   408      11.428   2.269   4.199  1.00  0.30
ATOM   1372  O   ILE   408      11.196   2.365   5.390  1.00  0.33
ATOM   1373  N   GLU   409      12.352   1.467   3.745  1.00  0.30
ATOM   1374  HN  GLU   409      12.522   1.420   2.781  1.00  0.29
ATOM   1375  CA  GLU   409      13.158   0.635   4.679  1.00  0.34
ATOM   1376  HA  GLU   409      12.522  -0.098   5.154  1.00  0.35
ATOM   1377  CB  GLU   409      14.265  -0.075   3.895  1.00  0.37
ATOM   1378  HB1 GLU   409      15.045   0.631   3.653  1.00  0.37
ATOM   1379  HB2 GLU   409      13.854  -0.482   2.982  1.00  0.36
ATOM   1380  CG  GLU   409      14.848  -1.205   4.742  1.00  0.44
ATOM   1381  HG1 GLU   409      14.100  -1.970   4.886  1.00  0.82
ATOM   1382  HG2 GLU   409      15.154  -0.814   5.702  1.00  0.75
ATOM   1383  CD  GLU   409      16.058  -1.807   4.026  1.00  1.01
ATOM   1384  OE1 GLU   409      15.856  -2.489   3.034  1.00  1.63
ATOM   1385  OE2 GLU   409      17.167  -1.575   4.480  1.00  1.75
ATOM   1386  C   GLU   409      13.778   1.543   5.740  1.00  0.36
```

Figure 8 (19 of 19)

```
ATOM   1387  O    GLU   409      13.902   1.179   6.892  1.00  0.39
ATOM   1388  N    GLU   410      14.151   2.733   5.357  1.00  0.35
ATOM   1389  HN   GLU   410      14.027   3.008   4.423  1.00  0.34
ATOM   1390  CA   GLU   410      14.744   3.678   6.341  1.00  0.38
ATOM   1391  HA   GLU   410      15.501   3.169   6.921  1.00  0.43
ATOM   1392  CB   GLU   410      15.369   4.865   5.605  1.00  0.43
ATOM   1393  HB1  GLU   410      14.846   5.771   5.873  1.00  1.11
ATOM   1394  HB2  GLU   410      15.294   4.707   4.539  1.00  0.91
ATOM   1395  CG   GLU   410      16.841   4.992   6.001  1.00  1.23
ATOM   1396  HG1  GLU   410      17.332   4.040   5.871  1.00  1.87
ATOM   1397  HG2  GLU   410      16.910   5.295   7.036  1.00  1.90
ATOM   1398  CD   GLU   410      17.520   6.039   5.116  1.00  1.74
ATOM   1399  OE1  GLU   410      18.332   6.788   5.635  1.00  2.28
ATOM   1400  OE2  GLU   410      17.218   6.073   3.934  1.00  2.35
ATOM   1401  C    GLU   410      13.635   4.174   7.268  1.00  0.35
ATOM   1402  O    GLU   410      13.846   4.401   8.443  1.00  0.38
ATOM   1403  N    ALA   411      12.447   4.331   6.747  1.00  0.32
ATOM   1404  HN   ALA   411      12.300   4.132   5.798  1.00  0.32
ATOM   1405  CA   ALA   411      11.315   4.797   7.594  1.00  0.33
ATOM   1406  HA   ALA   411      11.526   5.787   7.972  1.00  0.35
ATOM   1407  CB   ALA   411      10.032   4.825   6.761  1.00  0.32
ATOM   1408  HB1  ALA   411      10.193   4.295   5.833  1.00  1.08
ATOM   1409  HB2  ALA   411       9.761   5.848   6.549  1.00  1.12
ATOM   1410  HB3  ALA   411       9.235   4.348   7.313  1.00  0.93
ATOM   1411  C    ALA   411      11.137   3.827   8.760  1.00  0.35
ATOM   1412  O    ALA   411      10.725   4.202   9.839  1.00  0.41
ATOM   1413  N    LEU   412      11.444   2.578   8.545  1.00  0.35
ATOM   1414  HN   LEU   412      11.773   2.300   7.663  1.00  0.33
ATOM   1415  CA   LEU   412      11.293   1.574   9.636  1.00  0.40
ATOM   1416  HA   LEU   412      10.362   1.748  10.156  1.00  0.43
ATOM   1417  CB   LEU   412      11.291   0.153   9.049  1.00  0.42
ATOM   1418  HB1  LEU   412      10.803  -0.517   9.740  1.00  0.55
ATOM   1419  HB2  LEU   412      12.311  -0.170   8.899  1.00  0.42
ATOM   1420  CG   LEU   412      10.548   0.122   7.703  1.00  0.49
ATOM   1421  HG   LEU   412      11.140   0.627   6.954  1.00  1.00
ATOM   1422  CD1  LEU   412      10.332  -1.332   7.277  1.00  0.79
ATOM   1423  HD11 LEU   412      10.766  -1.489   6.301  1.00  1.34
ATOM   1424  HD12 LEU   412       9.274  -1.543   7.238  1.00  1.35
ATOM   1425  HD13 LEU   412      10.805  -1.990   7.991  1.00  1.42
ATOM   1426  CD2  LEU   412       9.186   0.814   7.836  1.00  0.82
ATOM   1427  HD21 LEU   412       8.762   0.590   8.804  1.00  1.47
ATOM   1428  HD22 LEU   412       8.524   0.457   7.061  1.00  1.27
ATOM   1429  HD23 LEU   412       9.314   1.882   7.736  1.00  1.40
ATOM   1430  C    LEU   412      12.456   1.718  10.620  1.00  0.44
ATOM   1431  O    LEU   412      12.340   1.393  11.785  1.00  0.50
ATOM   1432  N    CYS   413      13.577   2.203  10.160  1.00  0.44
ATOM   1433  HN   CYS   413      13.650   2.461   9.217  1.00  0.41
ATOM   1434  CA   CYS   413      14.746   2.369  11.070  1.00  0.51
ATOM   1435  HA   CYS   413      14.701   1.626  11.852  1.00  0.89
ATOM   1436  CB   CYS   413      16.041   2.196  10.274  1.00  1.35
ATOM   1437  HB1  CYS   413      16.798   2.856  10.671  1.00  1.97
ATOM   1438  HB2  CYS   413      15.862   2.436   9.237  1.00  1.82
ATOM   1439  SG   CYS   413      16.606   0.481  10.406  1.00  2.31
ATOM   1440  HG   CYS   413      16.332   0.143  11.261  1.00  2.68
ATOM   1441  C    CYS   413      14.713   3.767  11.691  1.00  1.45
ATOM   1442  O    CYS   413      15.731   4.411  11.846  1.00  2.03
END
```